

FIG. 1(a)

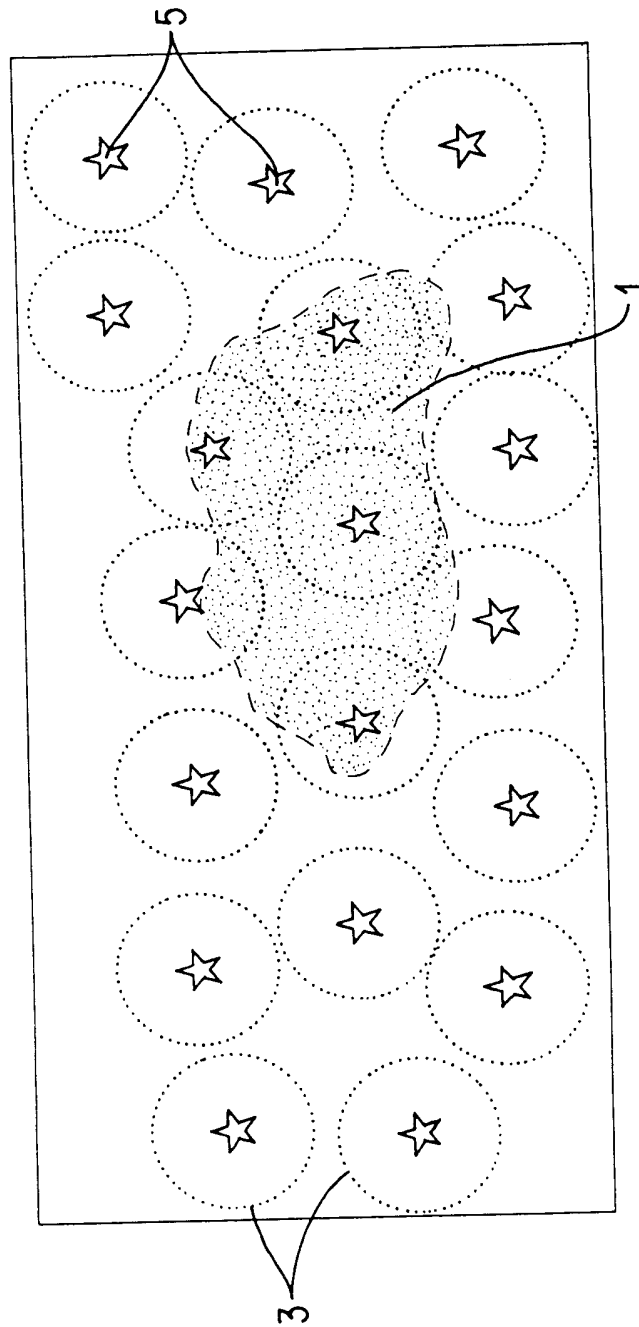


FIG. 1(b)

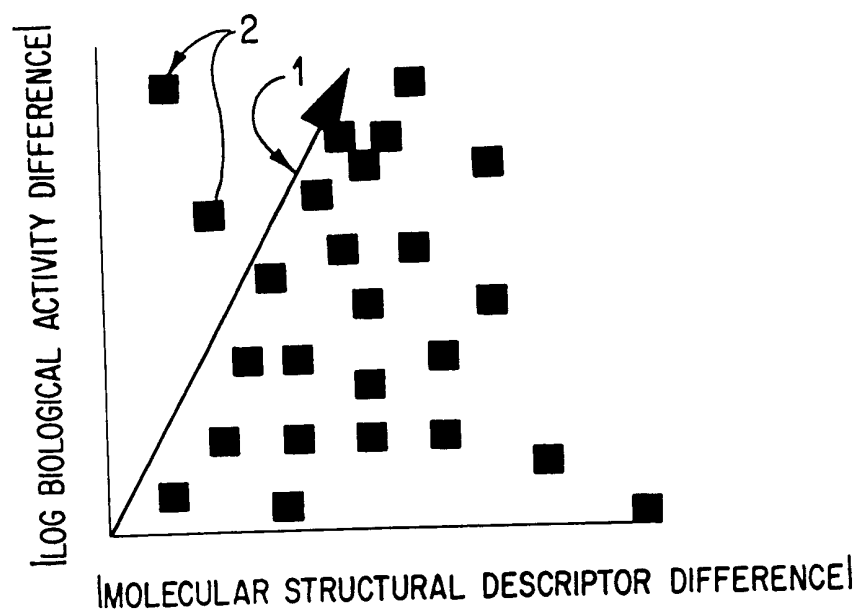


FIG. 2

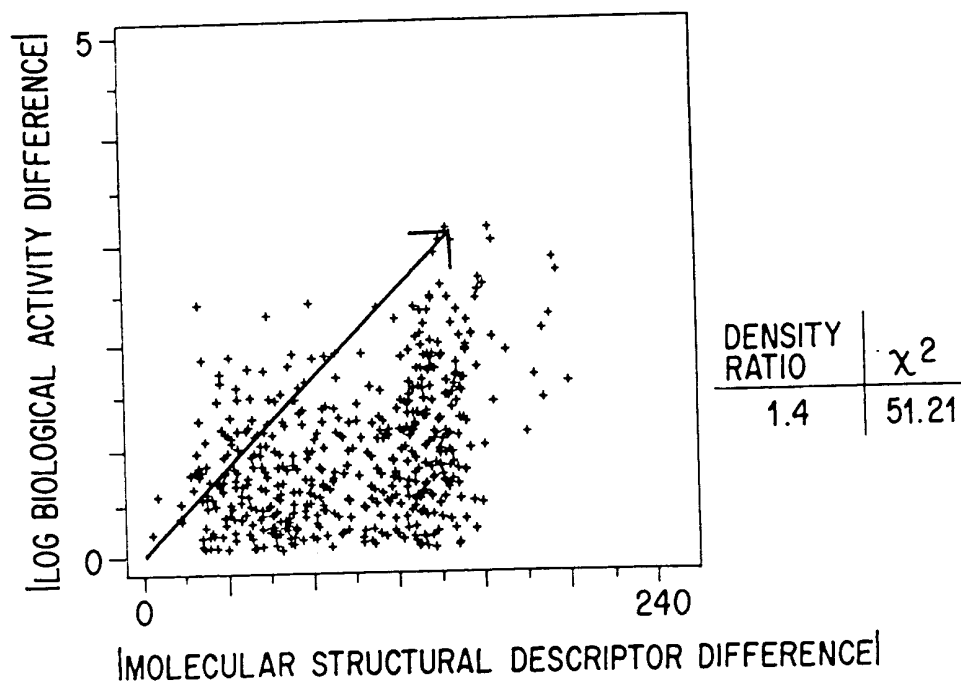
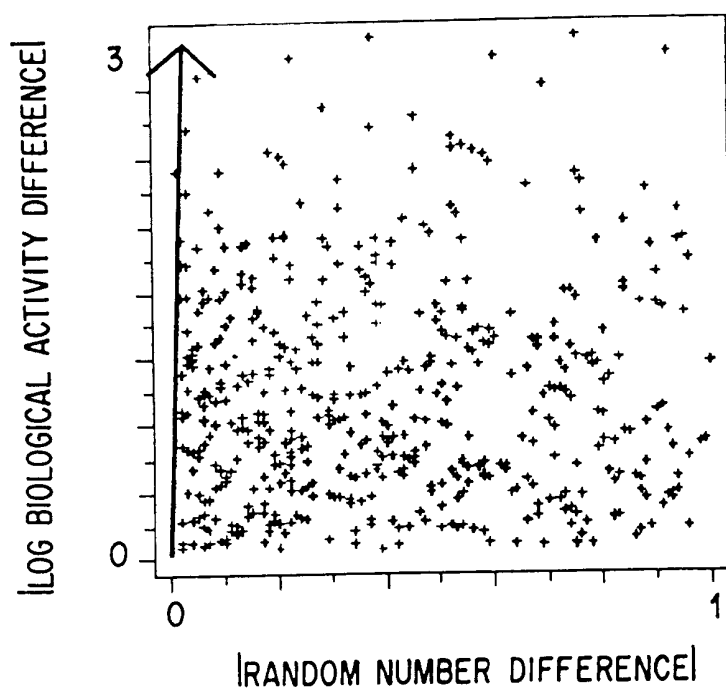
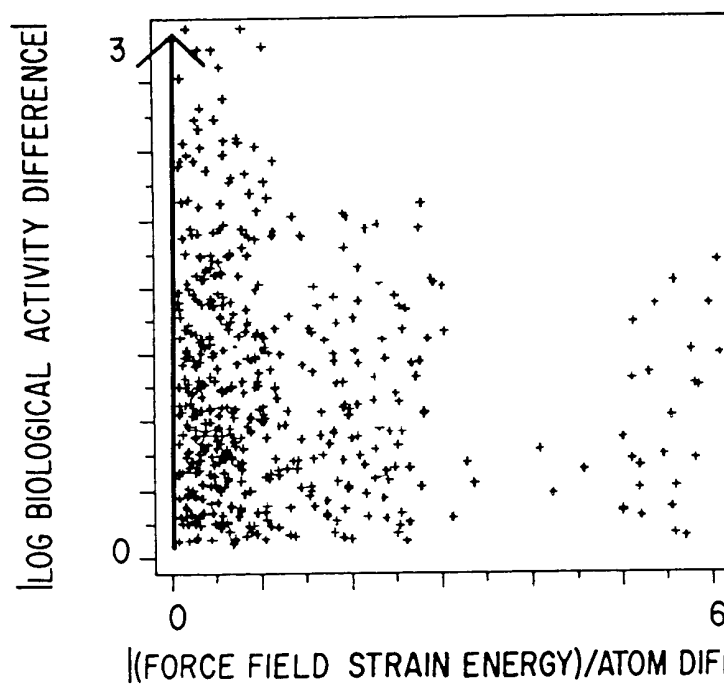


FIG. 3



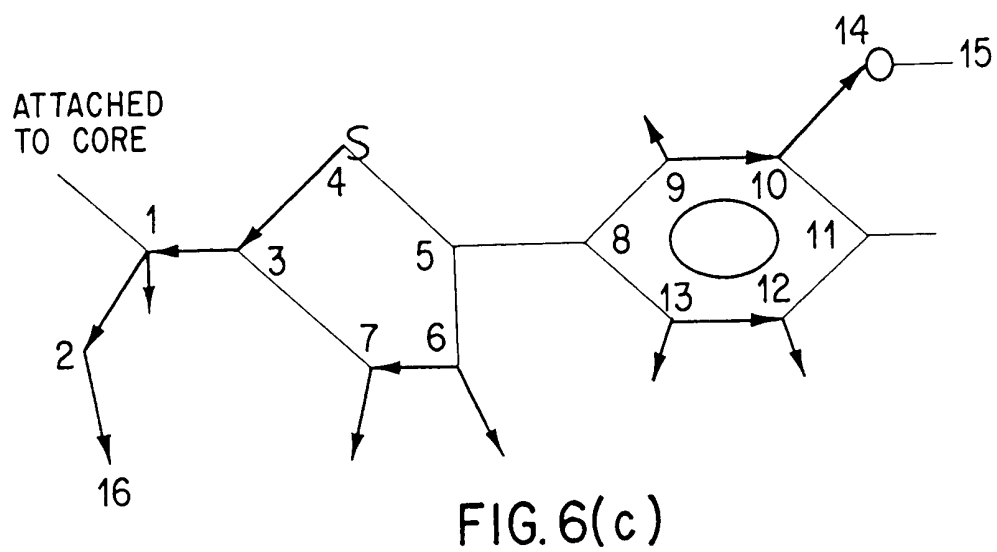
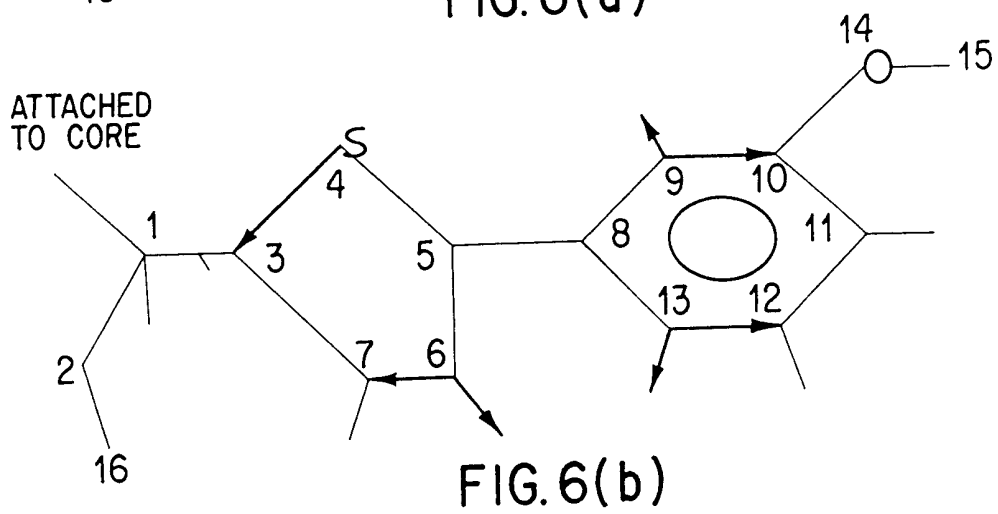
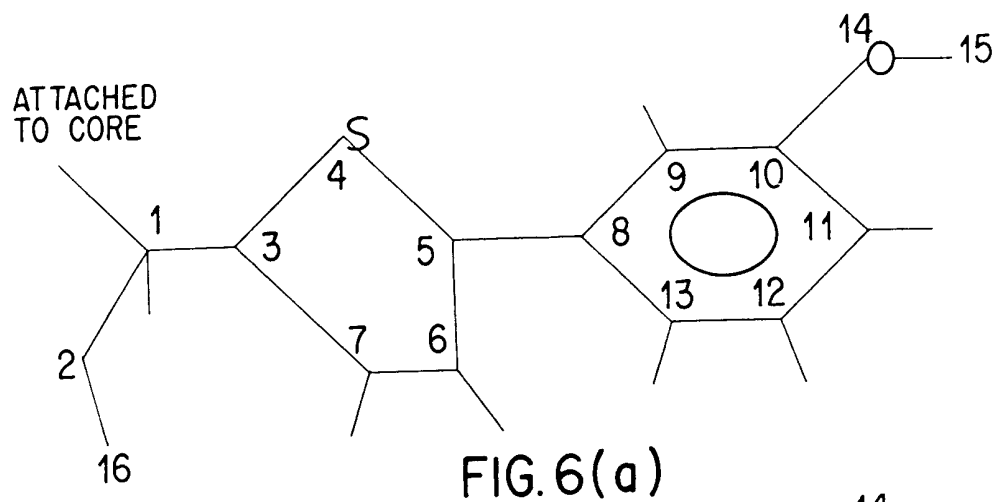
DENSITY RATIO	$\chi^2$
1.00	0.00

FIG. 4



DENSITY RATIO	$\chi^2$
0.96	0.46

FIG. 5



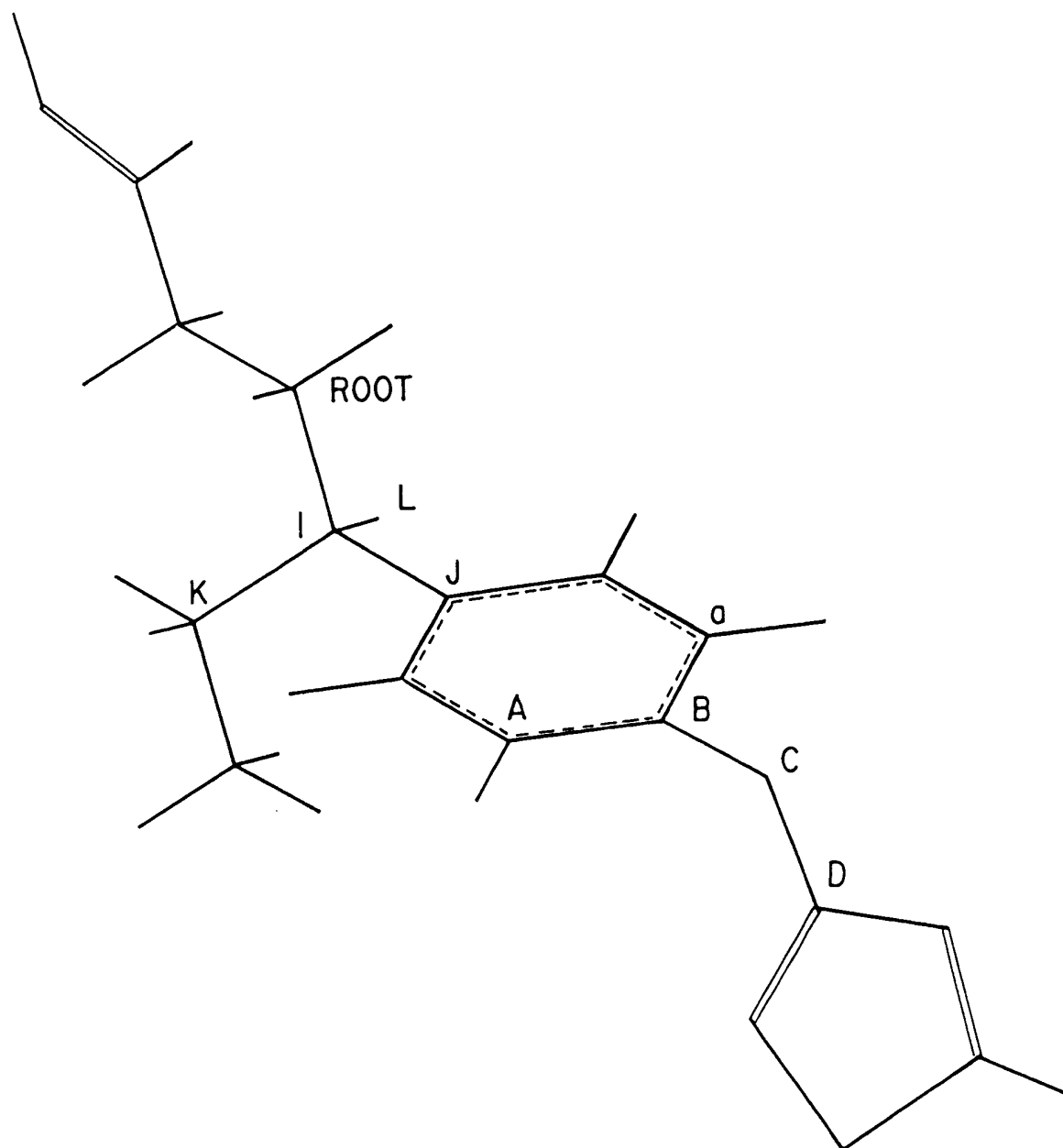


FIG. 6(d)

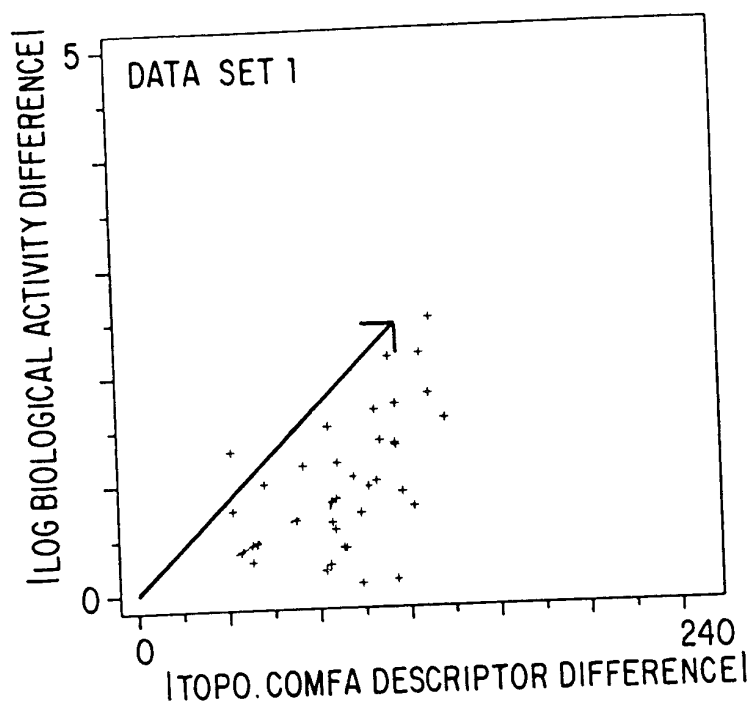


FIG.7(a)

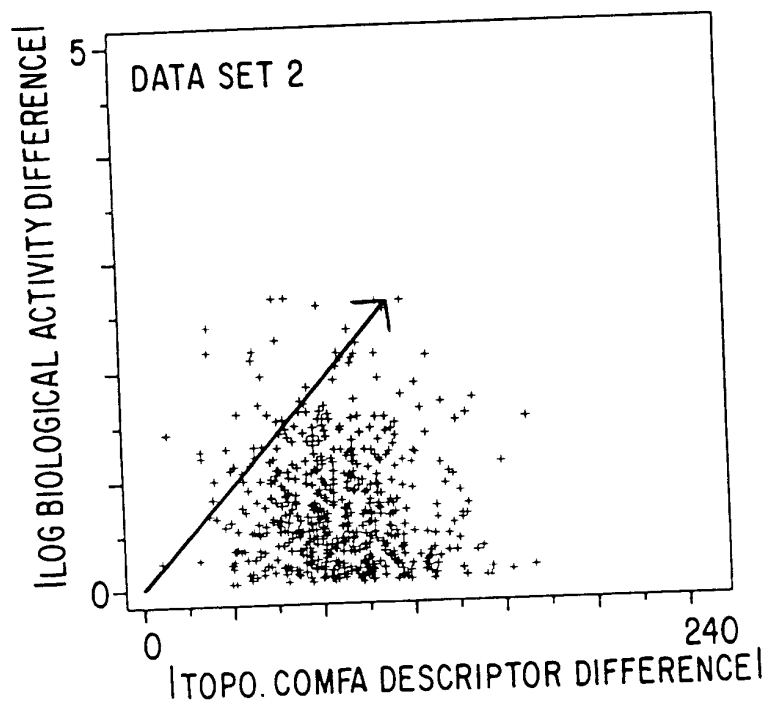


FIG.7(b)

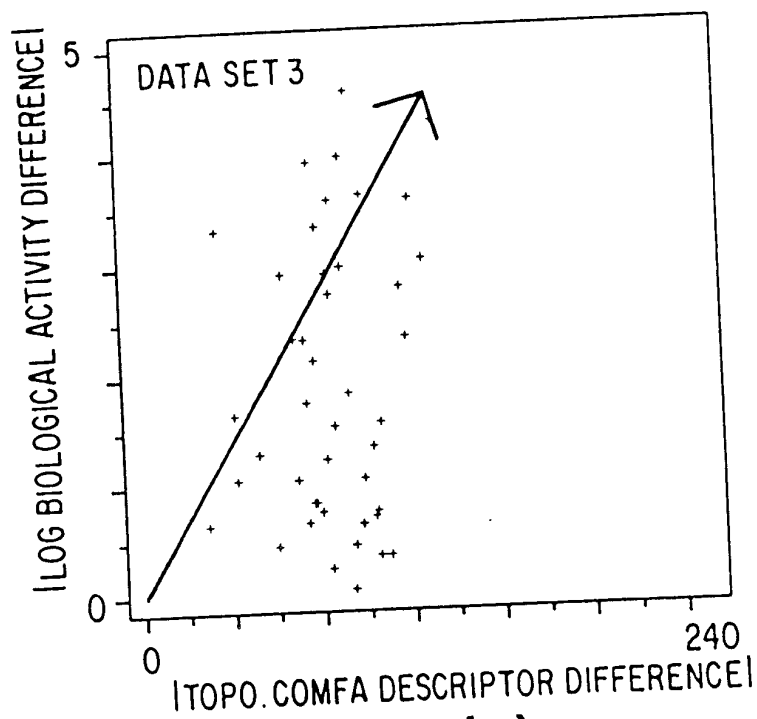


FIG. 7(c)

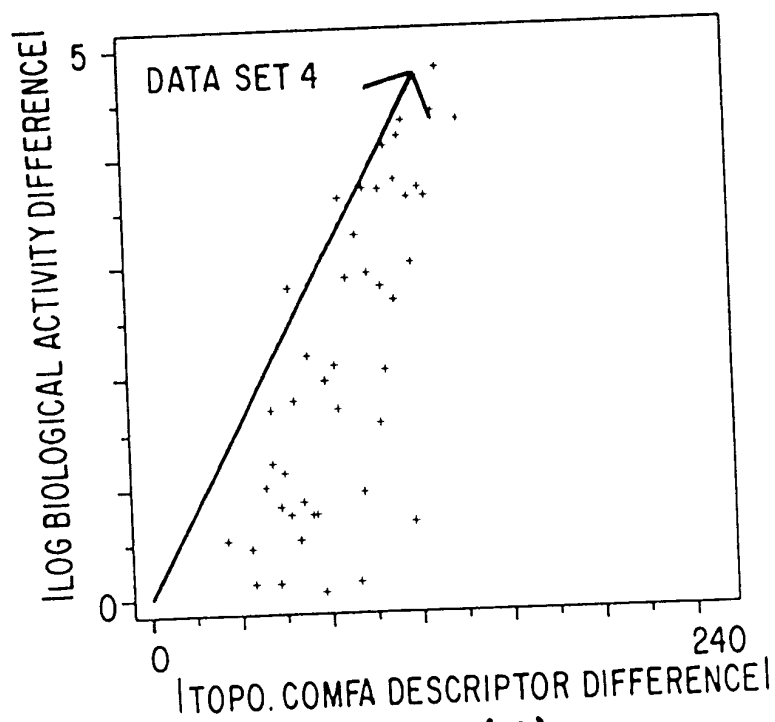


FIG. 7(d)



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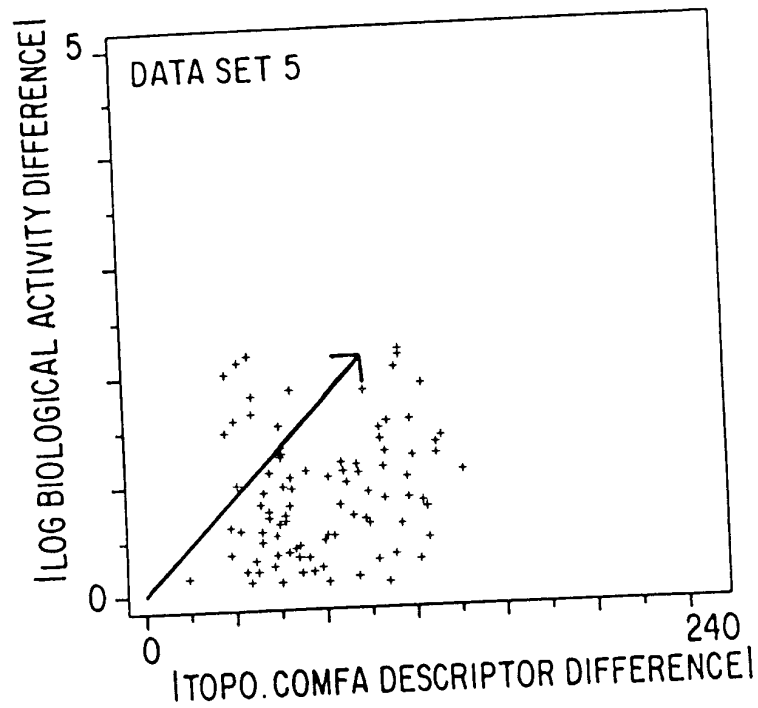


FIG.7(e)

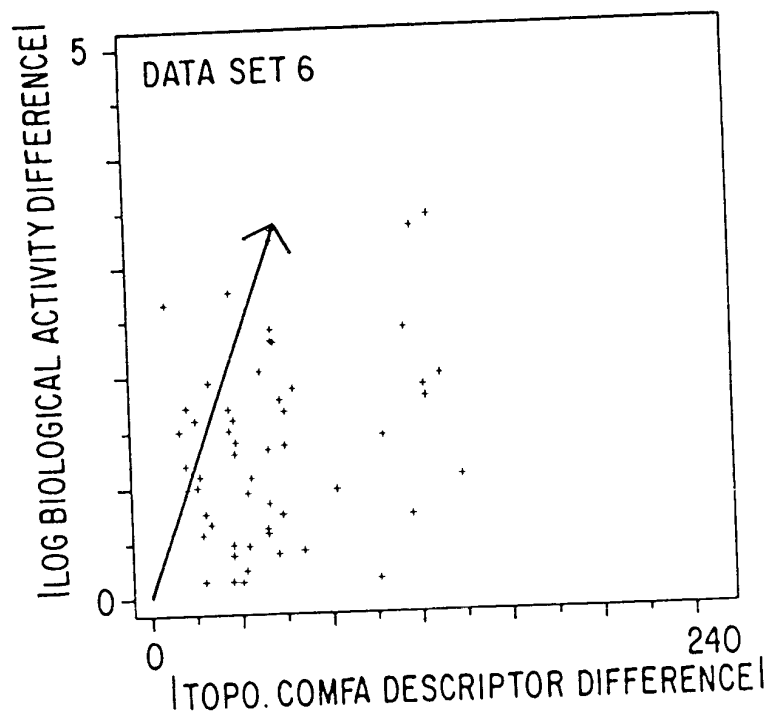


FIG.7(f)

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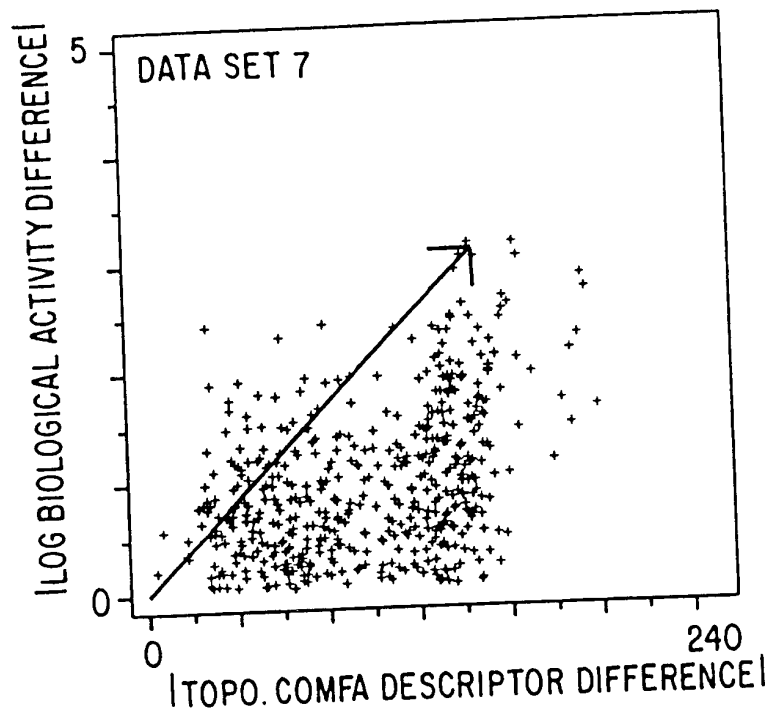


FIG.7(g)

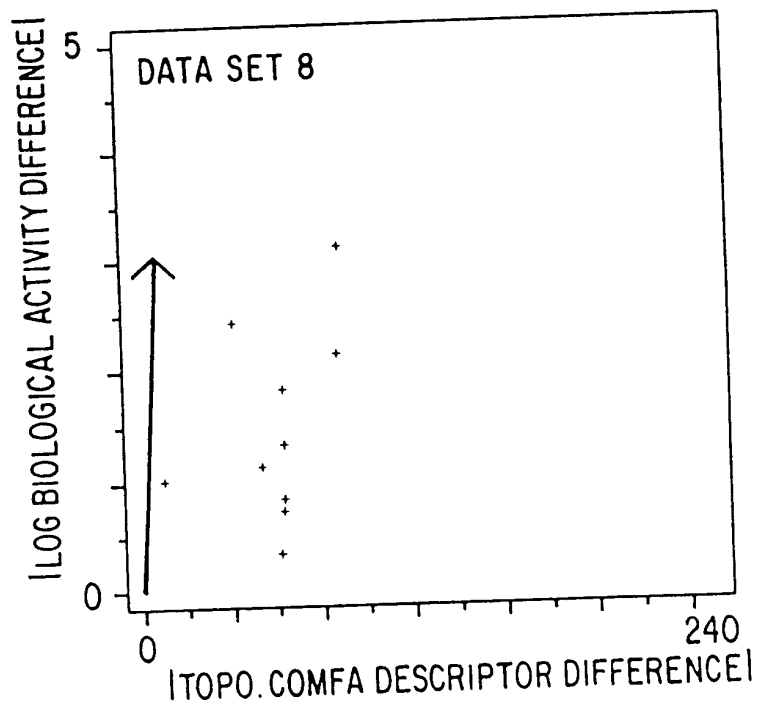


FIG.7(h)

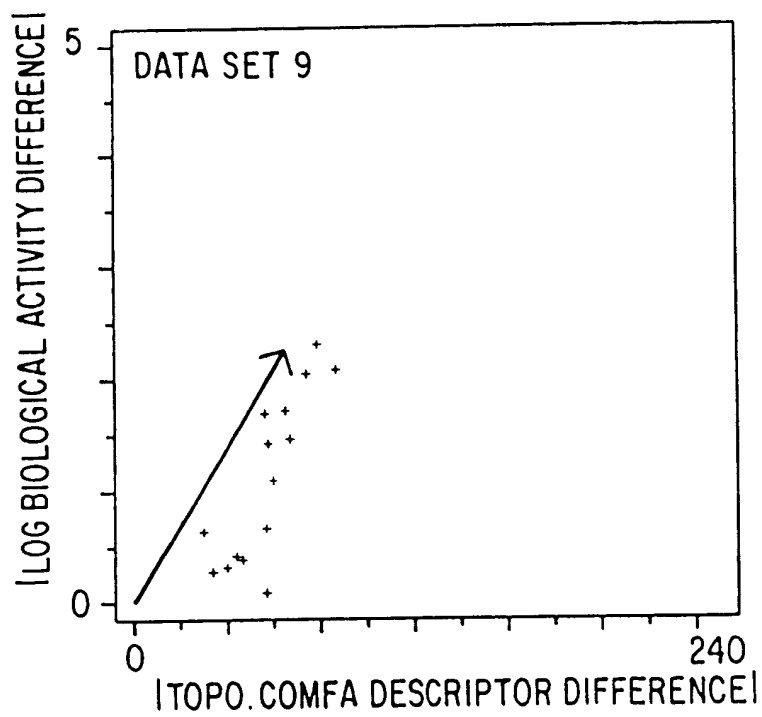


FIG.7(i)

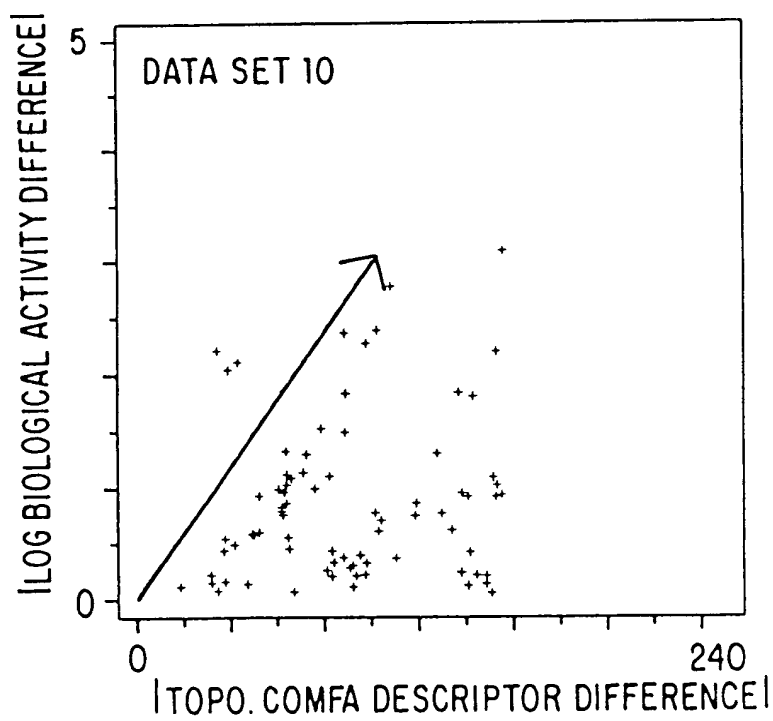


FIG.7(j)

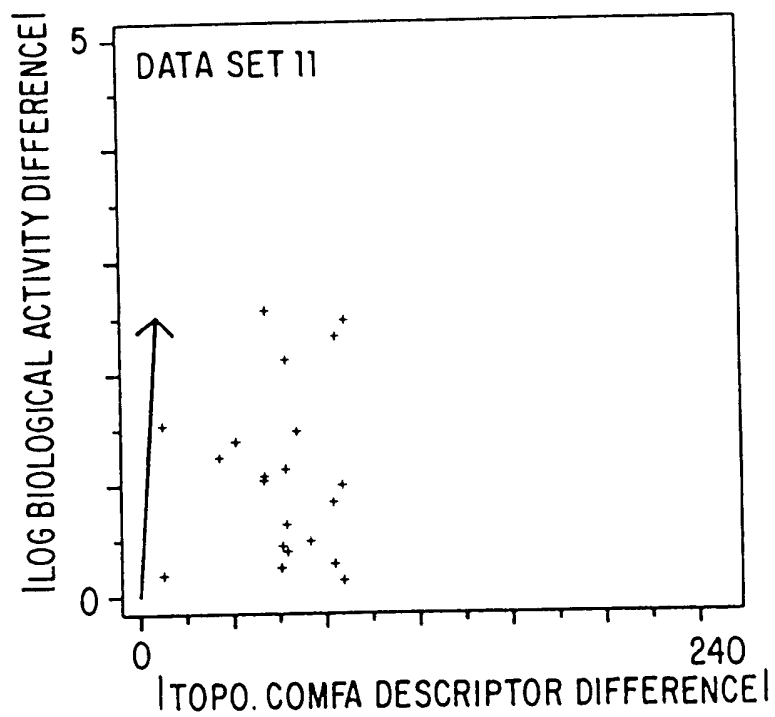


FIG.7(k)

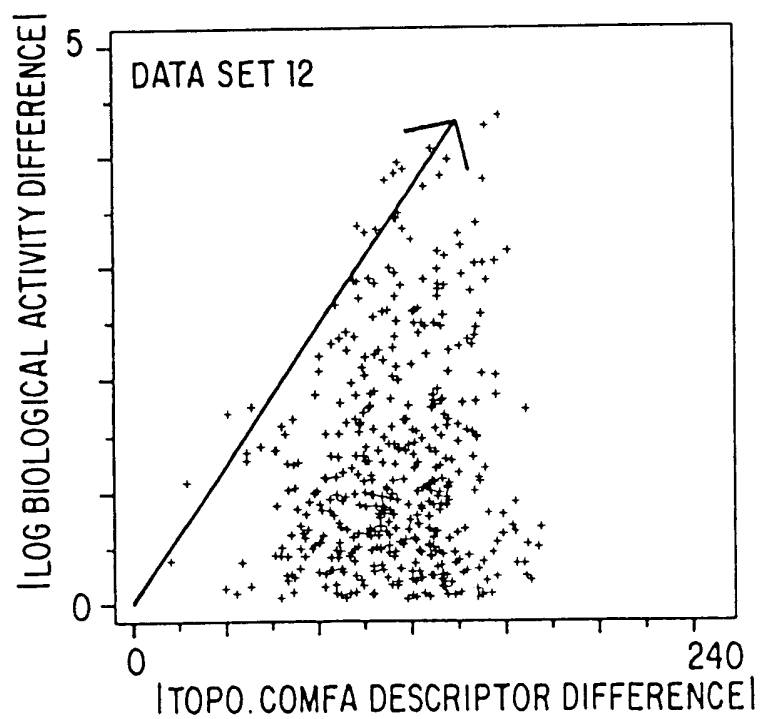


FIG.7(l)

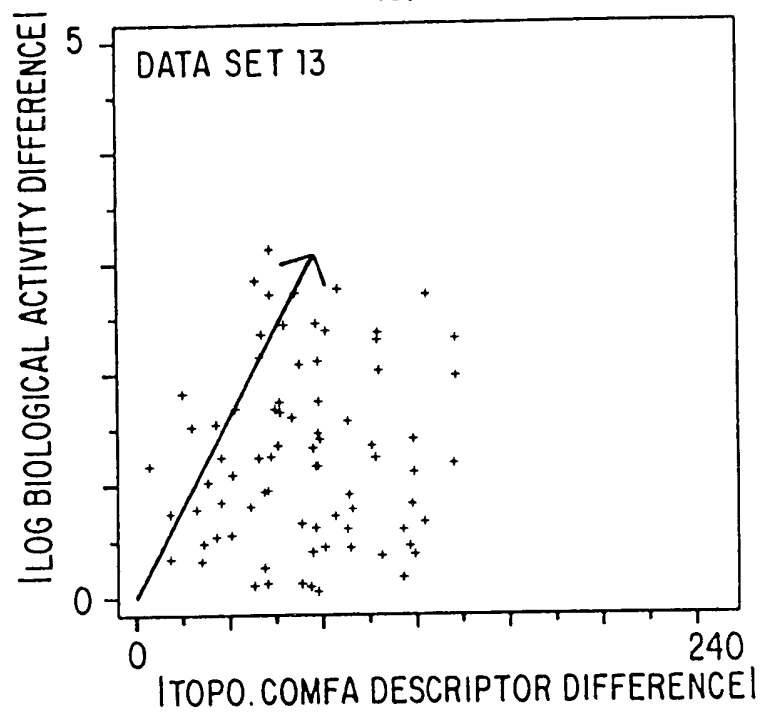


FIG. 7(m)

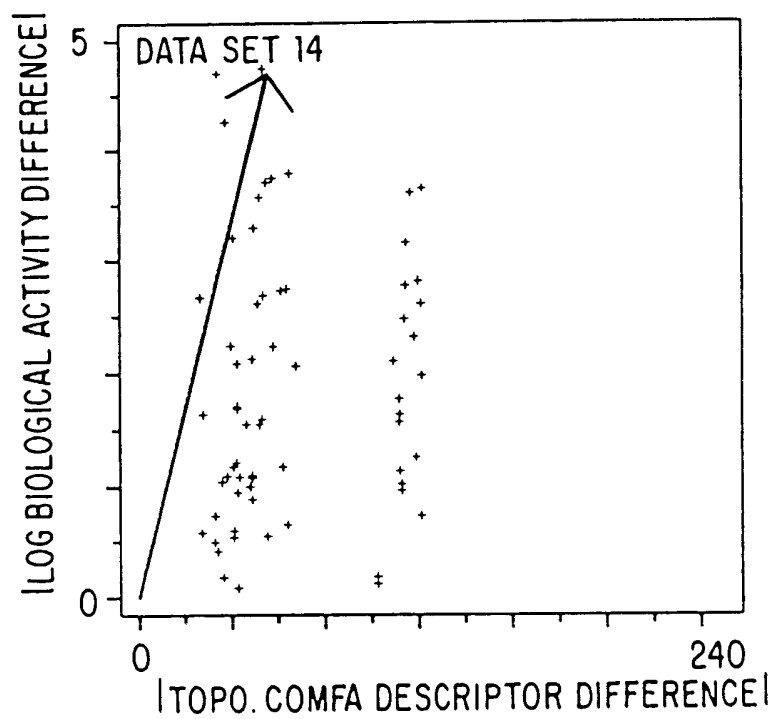


FIG. 7(n)

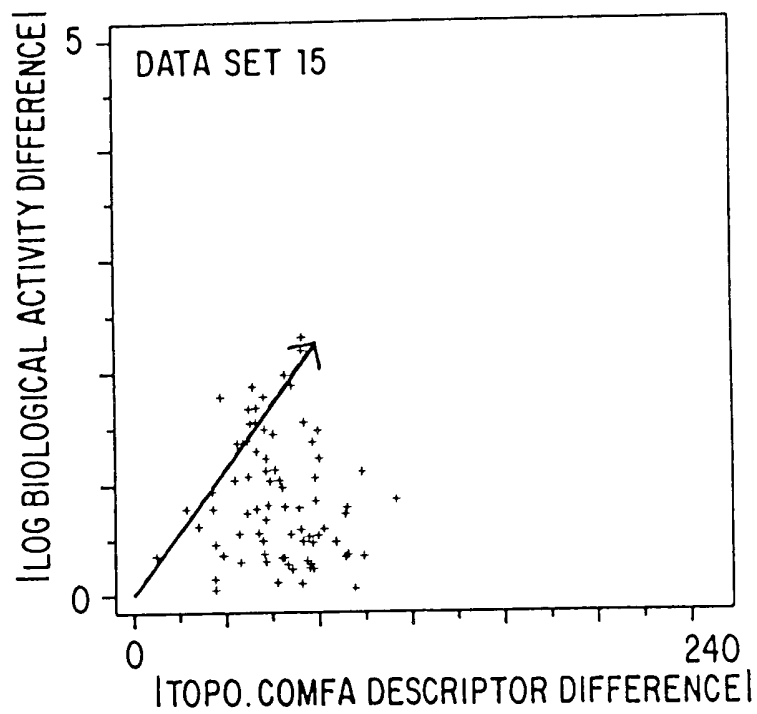


FIG.7(o)

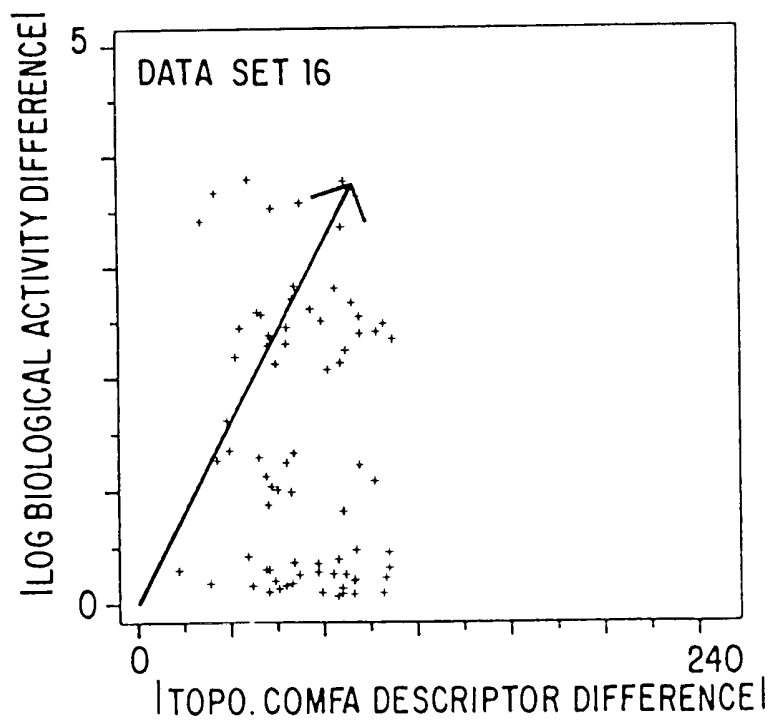


FIG.7(p)

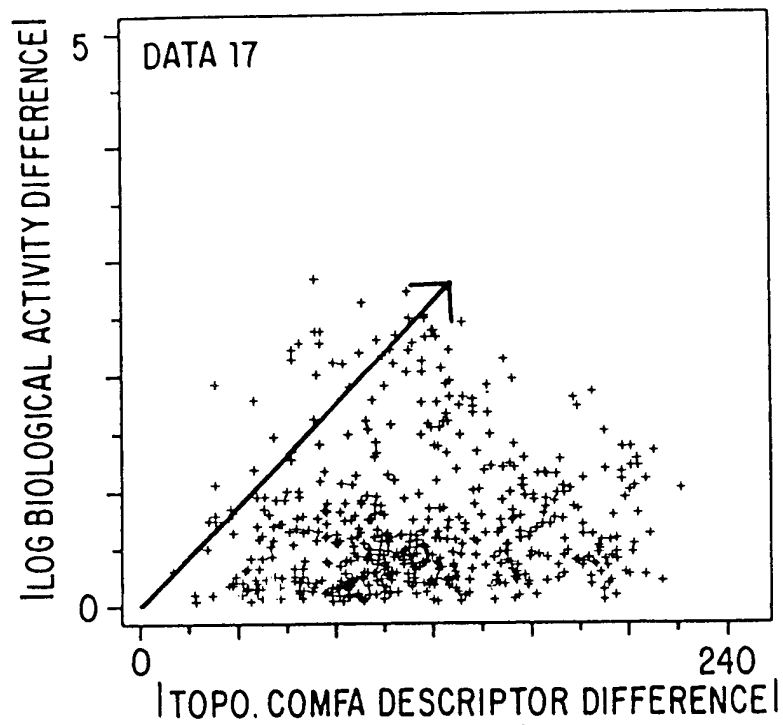


FIG.7(q)

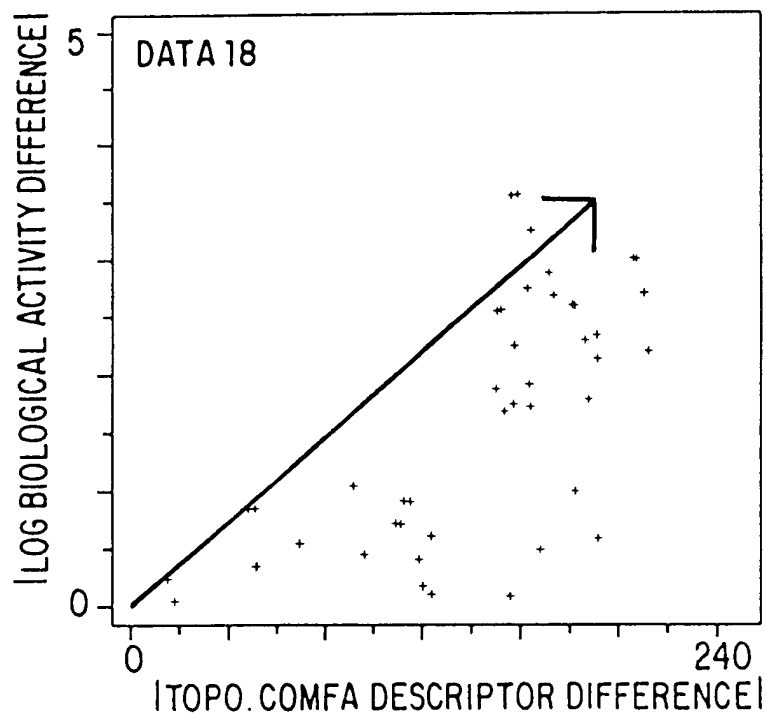


FIG.7(r)

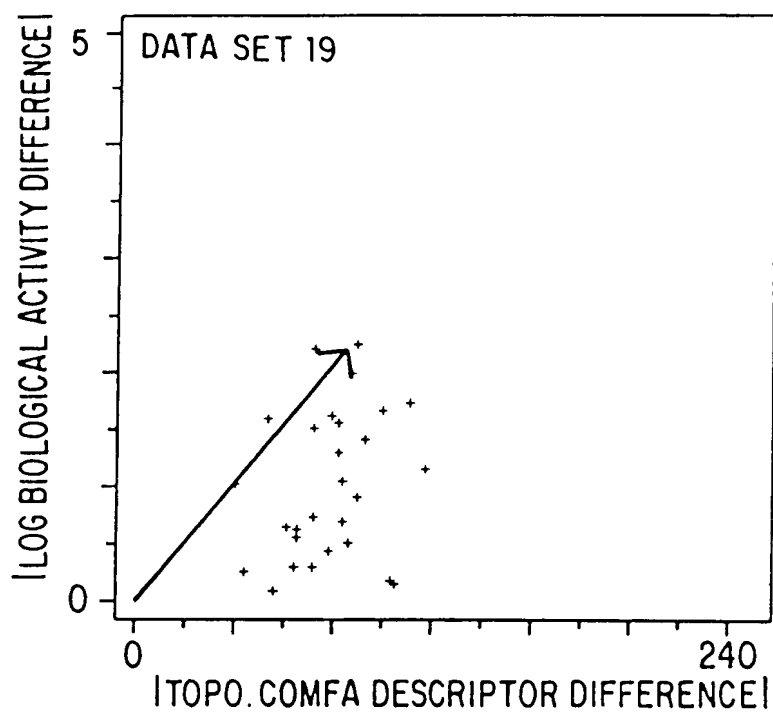


FIG. 7(s)

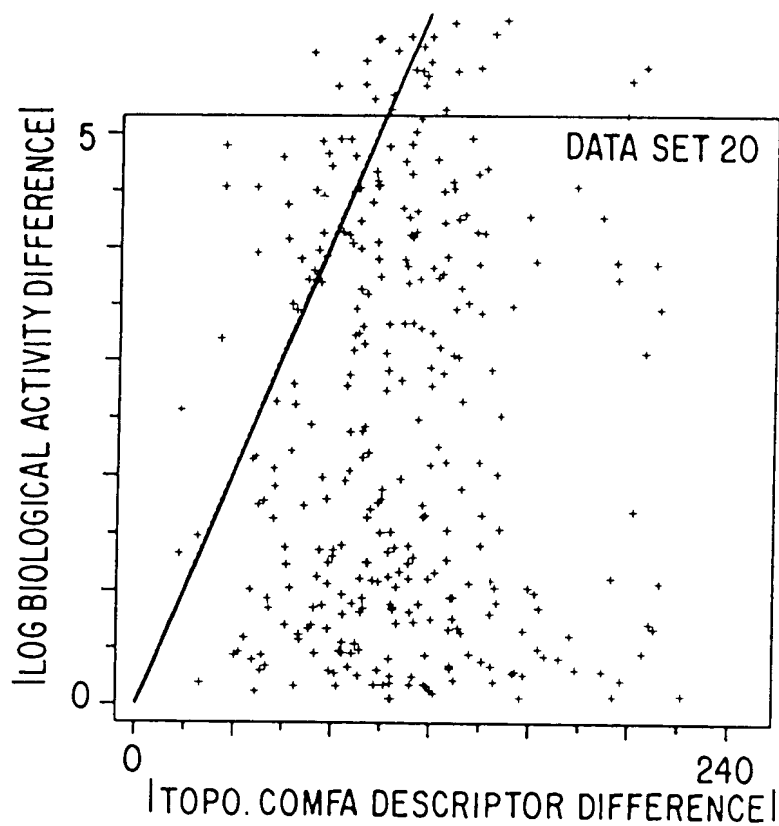
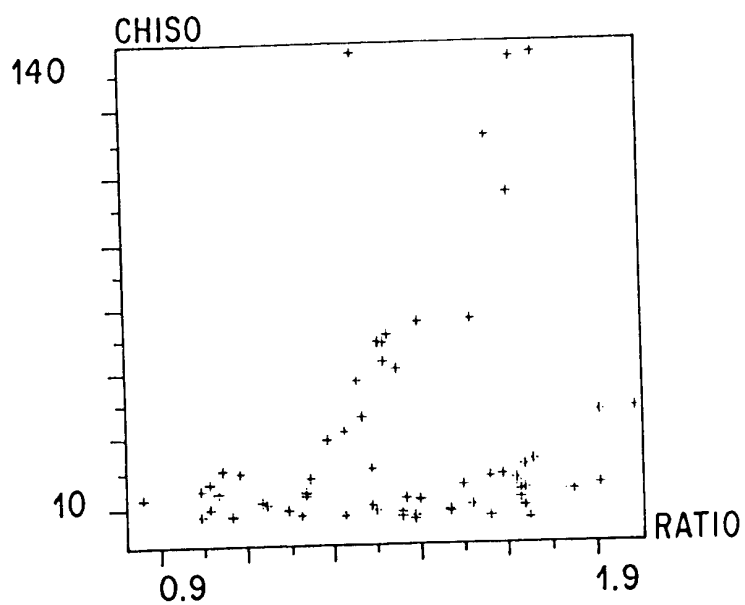


FIG. 7(t)

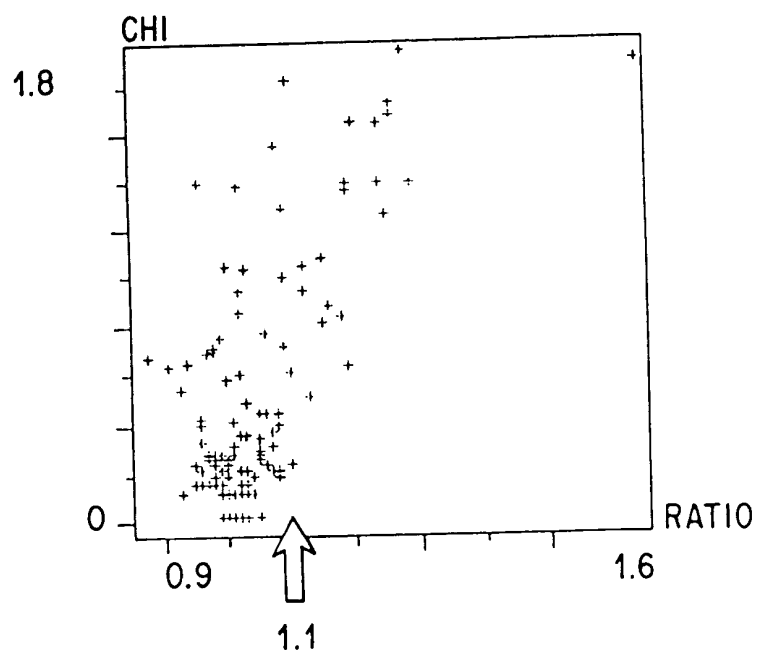


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1.1

FIG. 8(a)



1.1

FIG. 8(b)

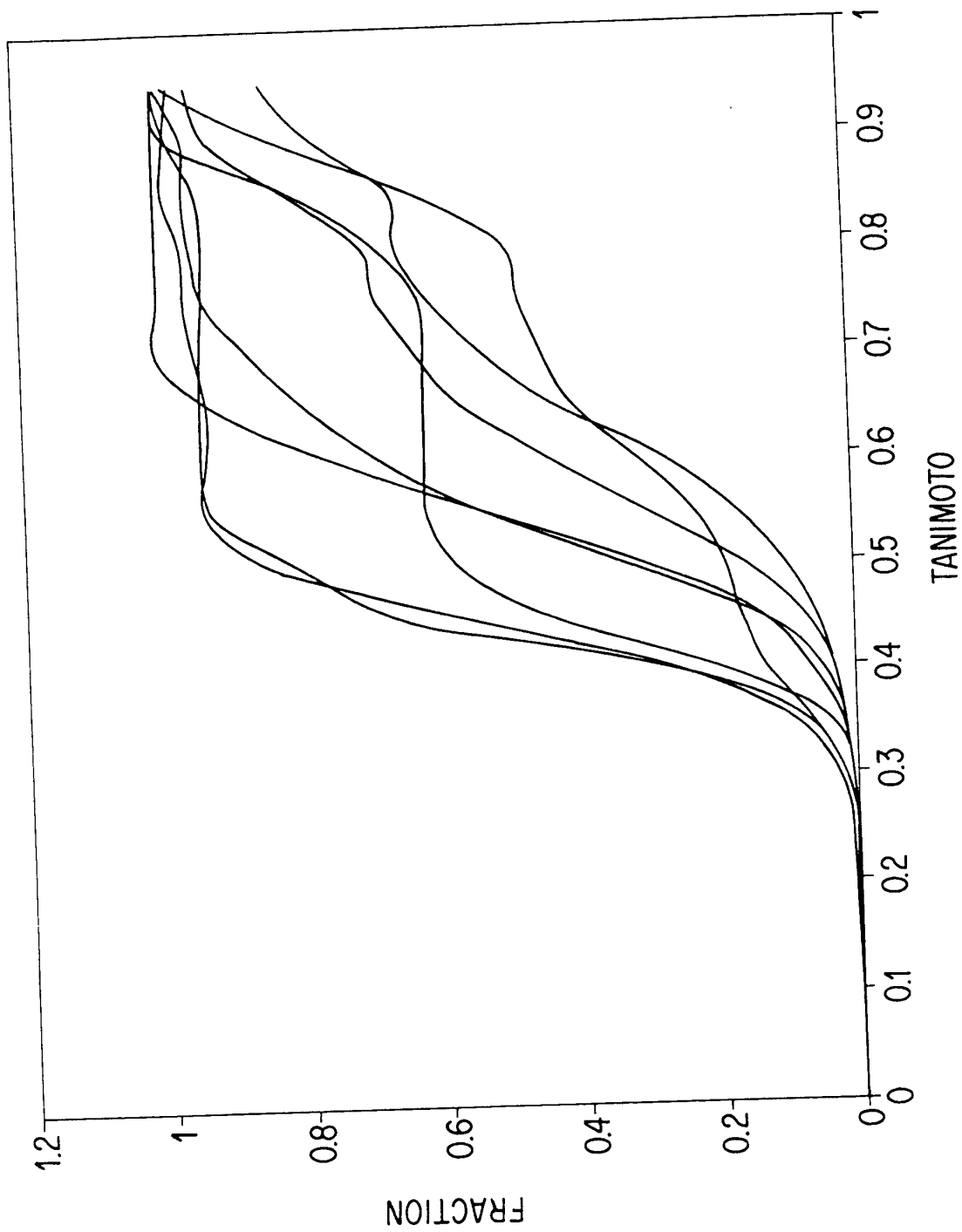


FIG. 9(a)

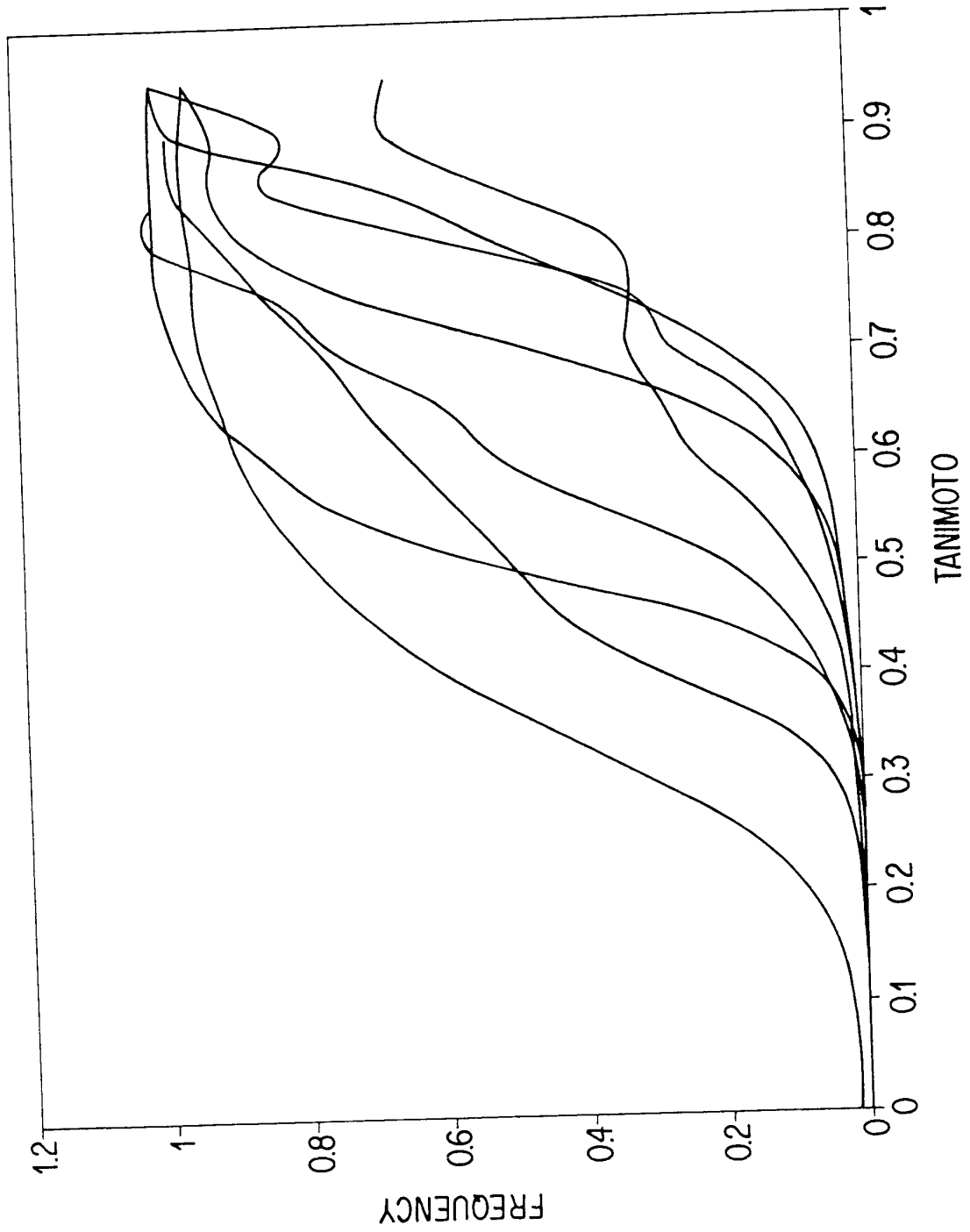
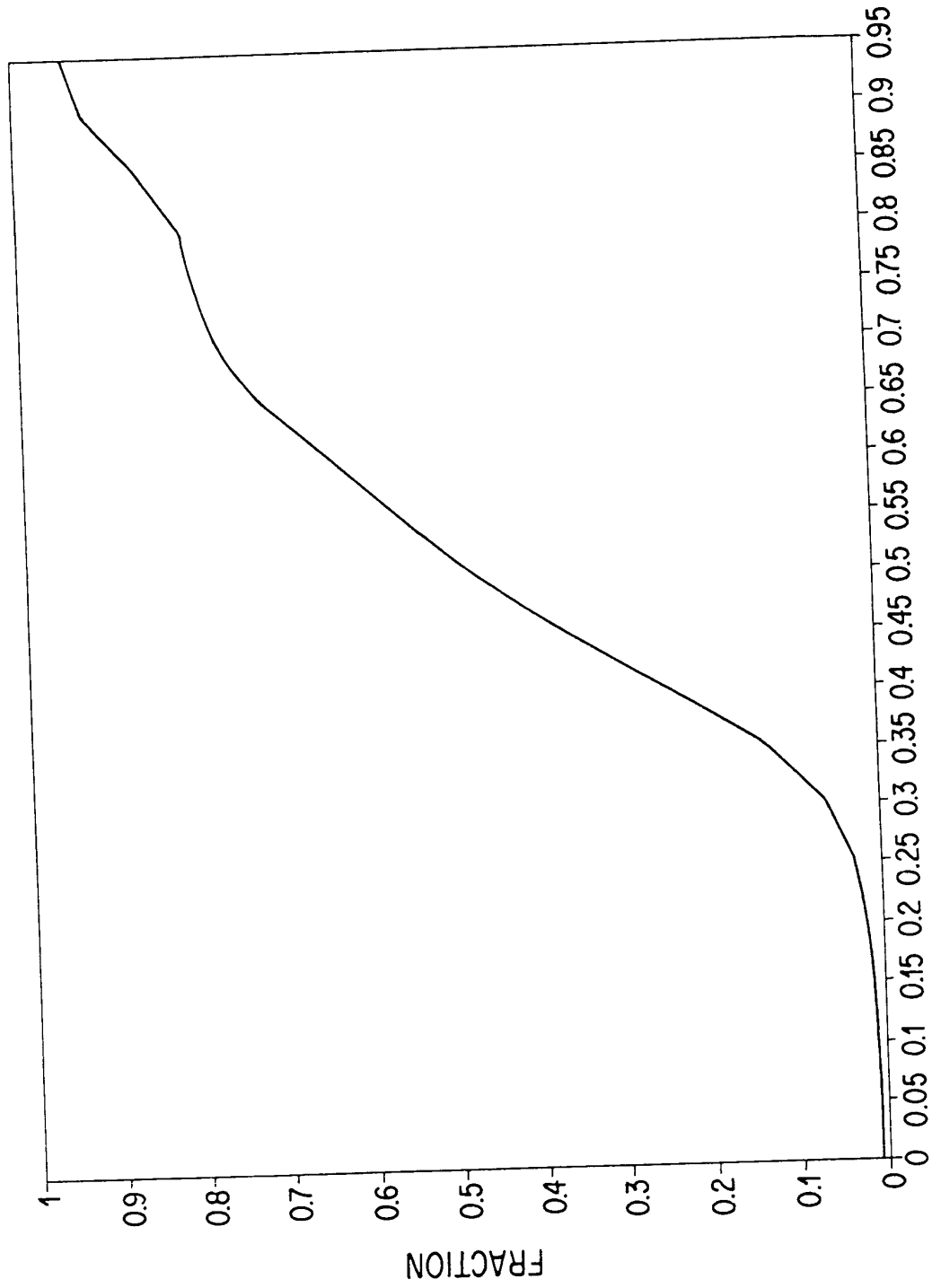


FIG. 9(b)



TANIMOTO

FIG. 9(c)

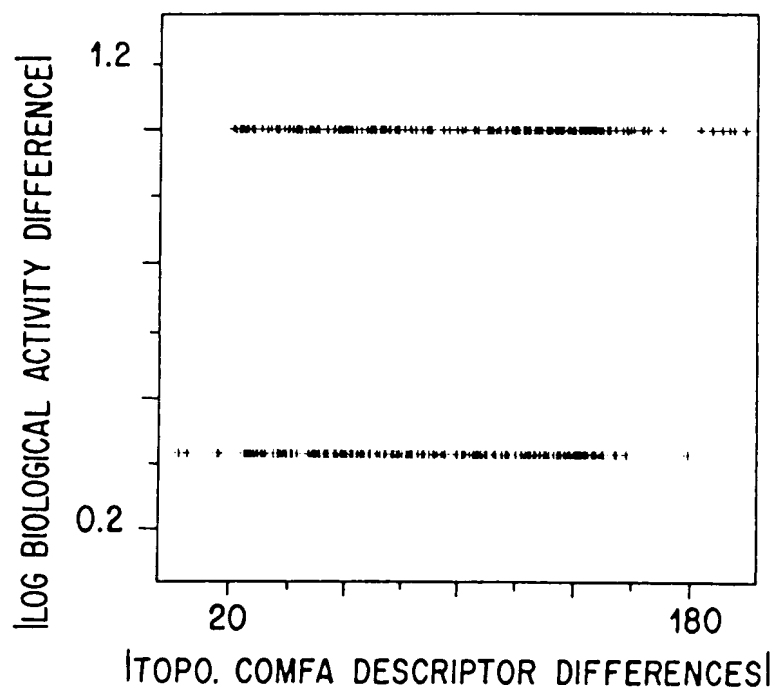


FIG.10(a)

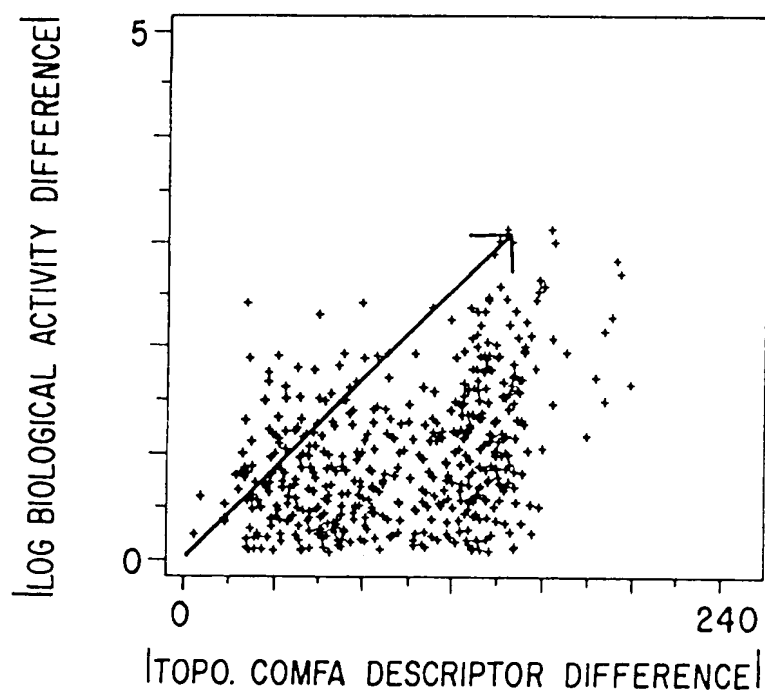


FIG.10(b)

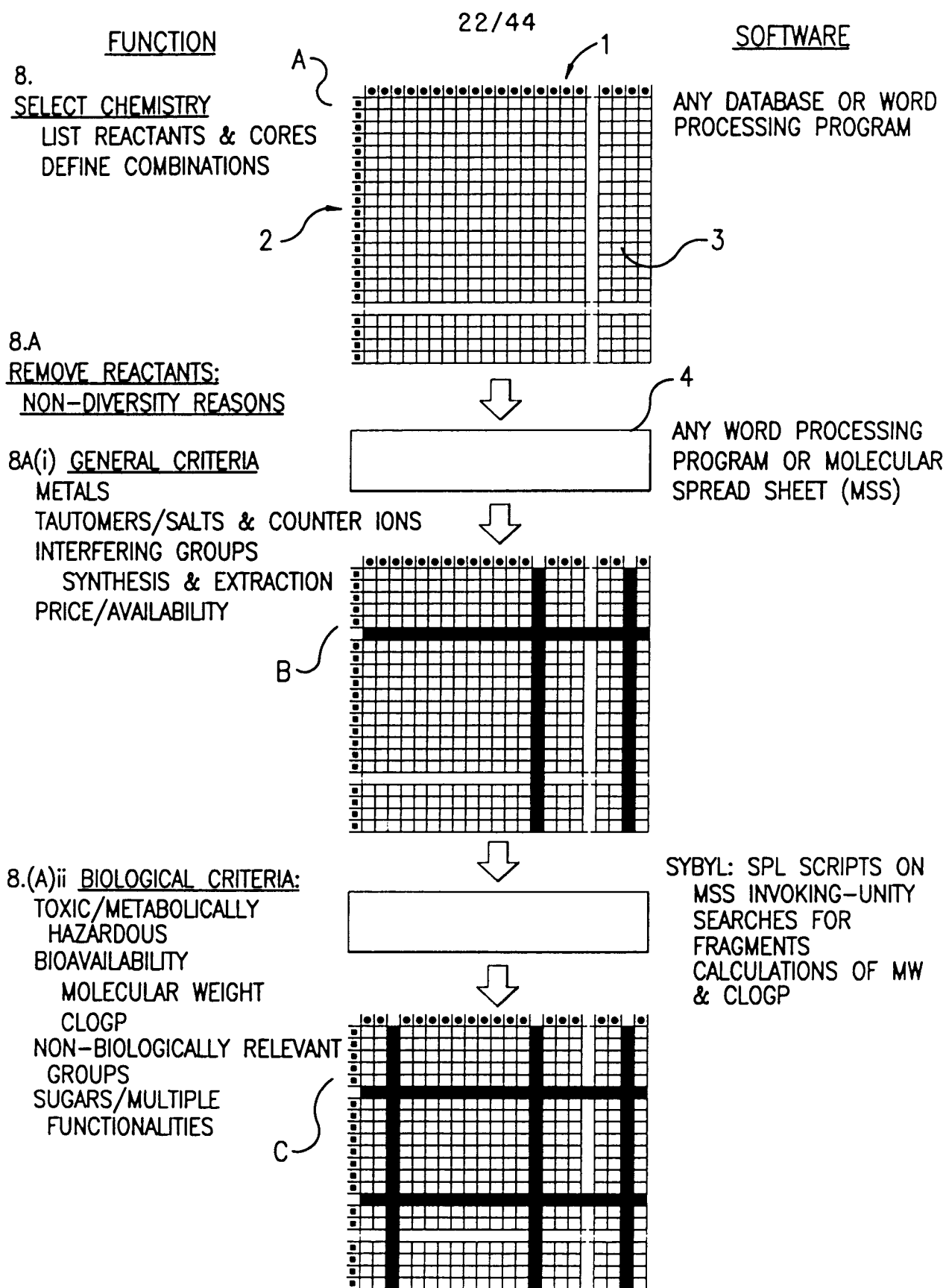


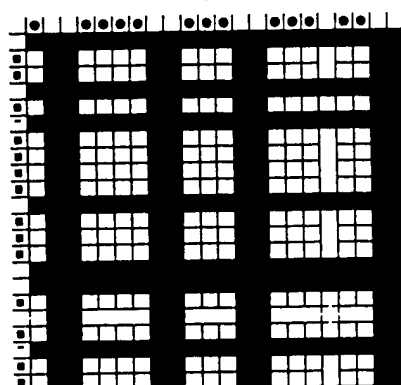
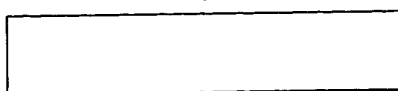
FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION  
 TOPOMERIC CONFORMER  
 ALIGNMENT  
 CoMFA FIELD GENERATION:  
 HYDROGEN BOND FIELD  
 GENERATION  
 ROTATABLE BOND FIELD  
 ATTENUATION  
 CALCULATE FIELD  
 DIFFERENCES  
 CLUSTER  
 REACTANT SELECTION FROM  
 EACH CLUSTER

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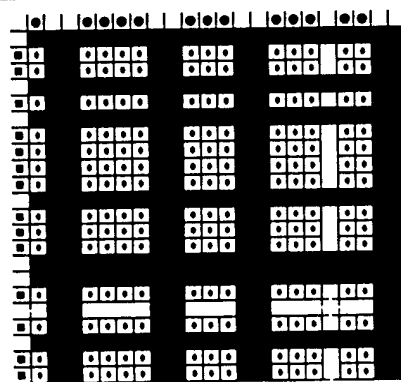
SYBYL: SELECTOR &  
 CONCORD 3.2.1  
 SPECIALIZED SOFTWARE:  
 APPENDIX "A"  
 (SYBYL: CoMFA  
 STERIC & MSS)

SYBYL: HIERCHICAL  
 CLUSTER - MSS  
 SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS

E



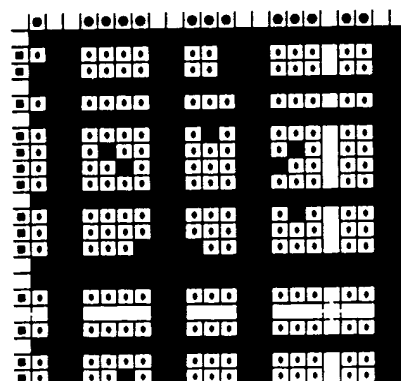
SYBYL: LEGION MSS

8D

REMOVE PRODUCTS:NON-DIVERSITY REASONS

GENERAL CRITERIA:

F



SYBYL: SPL SCRIPTS  
 ON MSS



FIG.11(b)

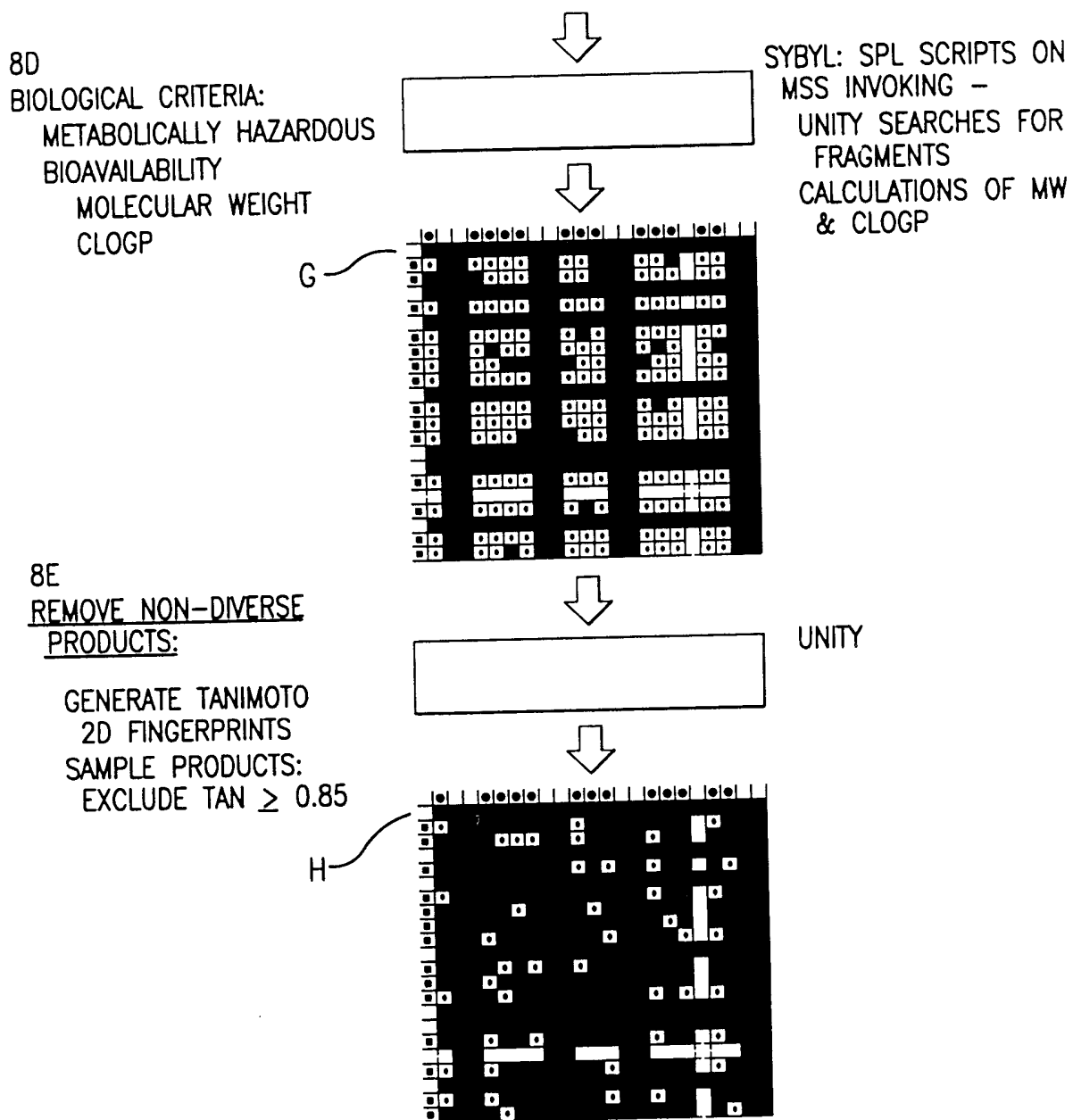


FIG.11(c)





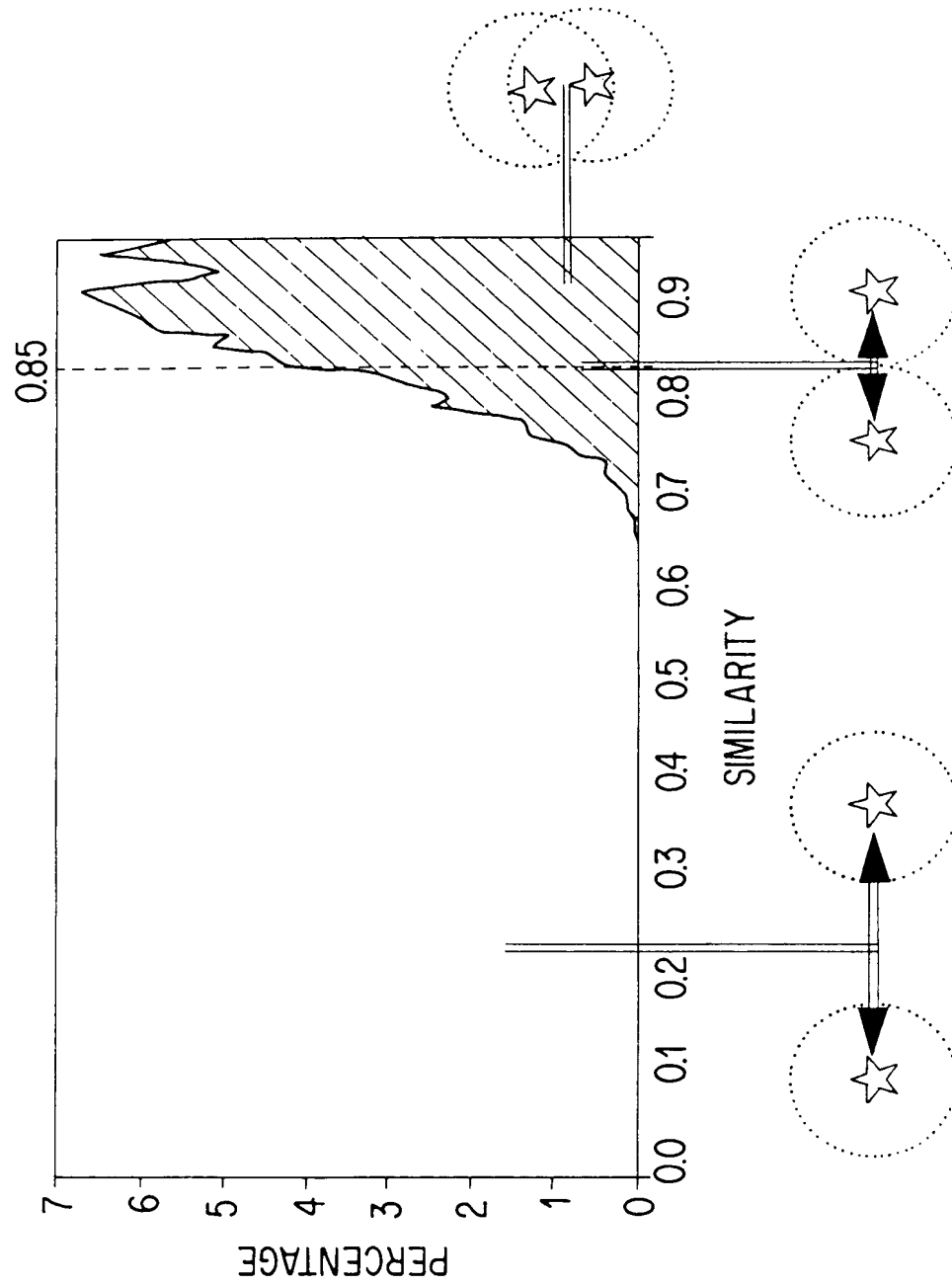


FIG. 13

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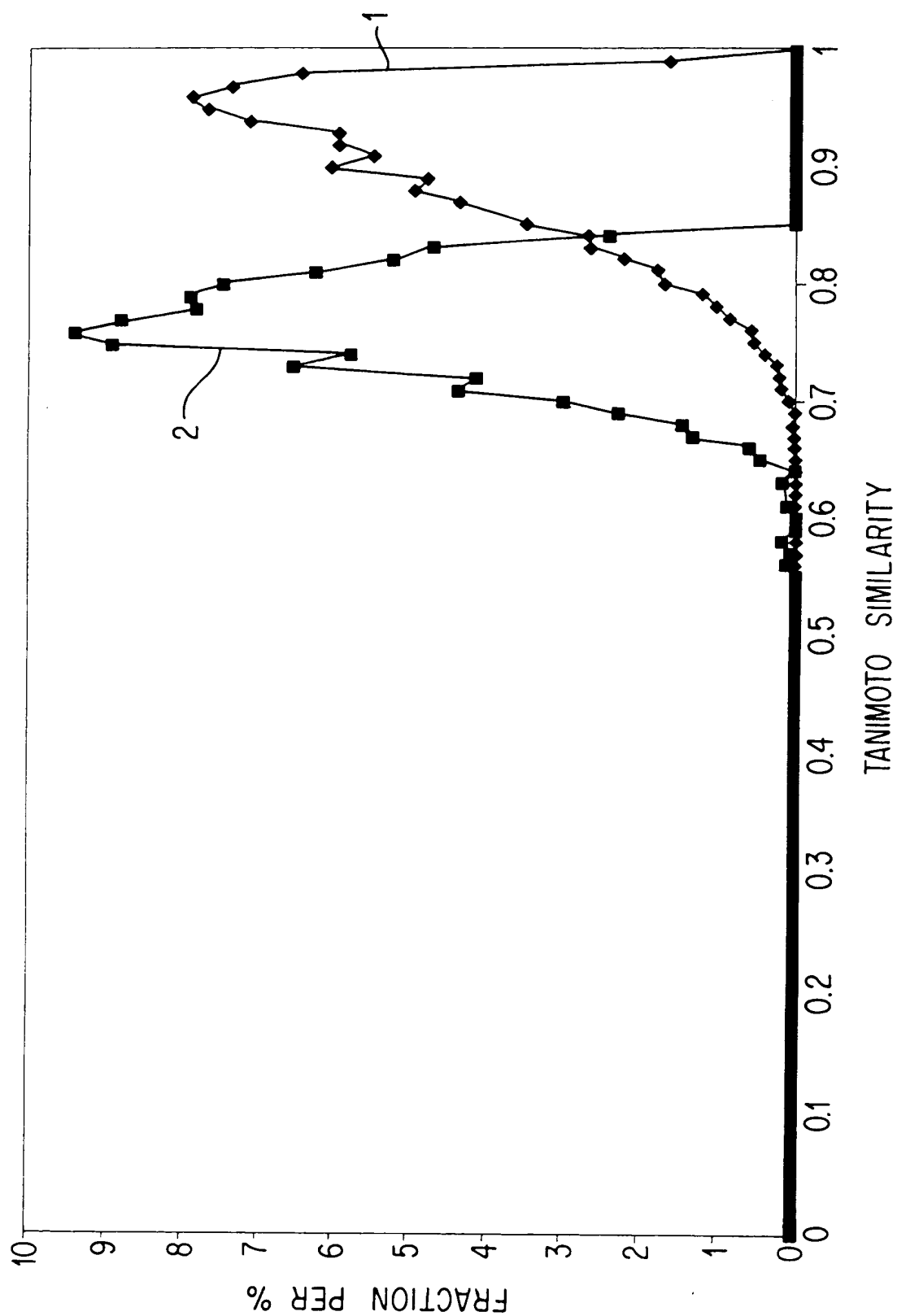


FIG. 14

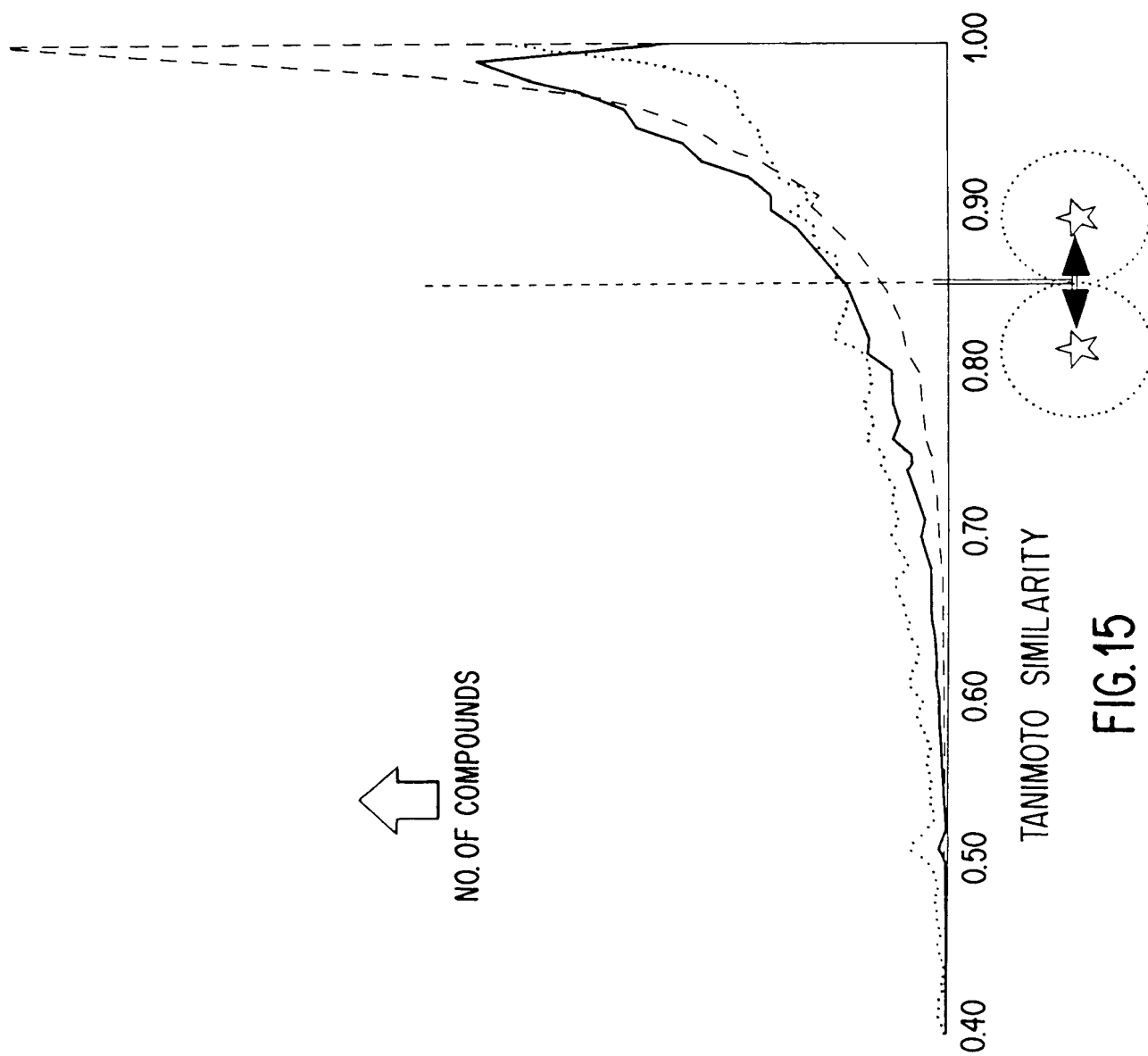


FIG. 15

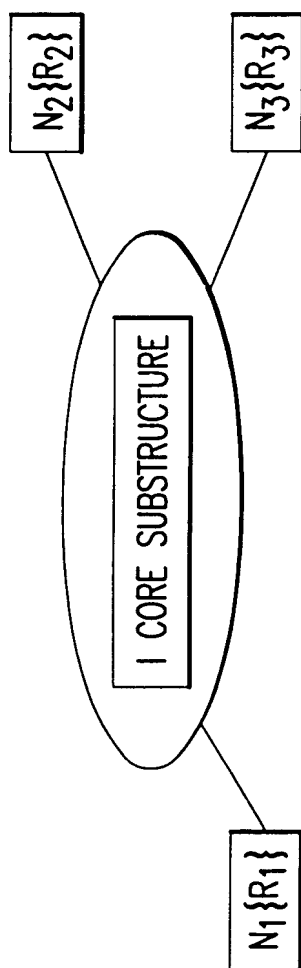


FIG.16

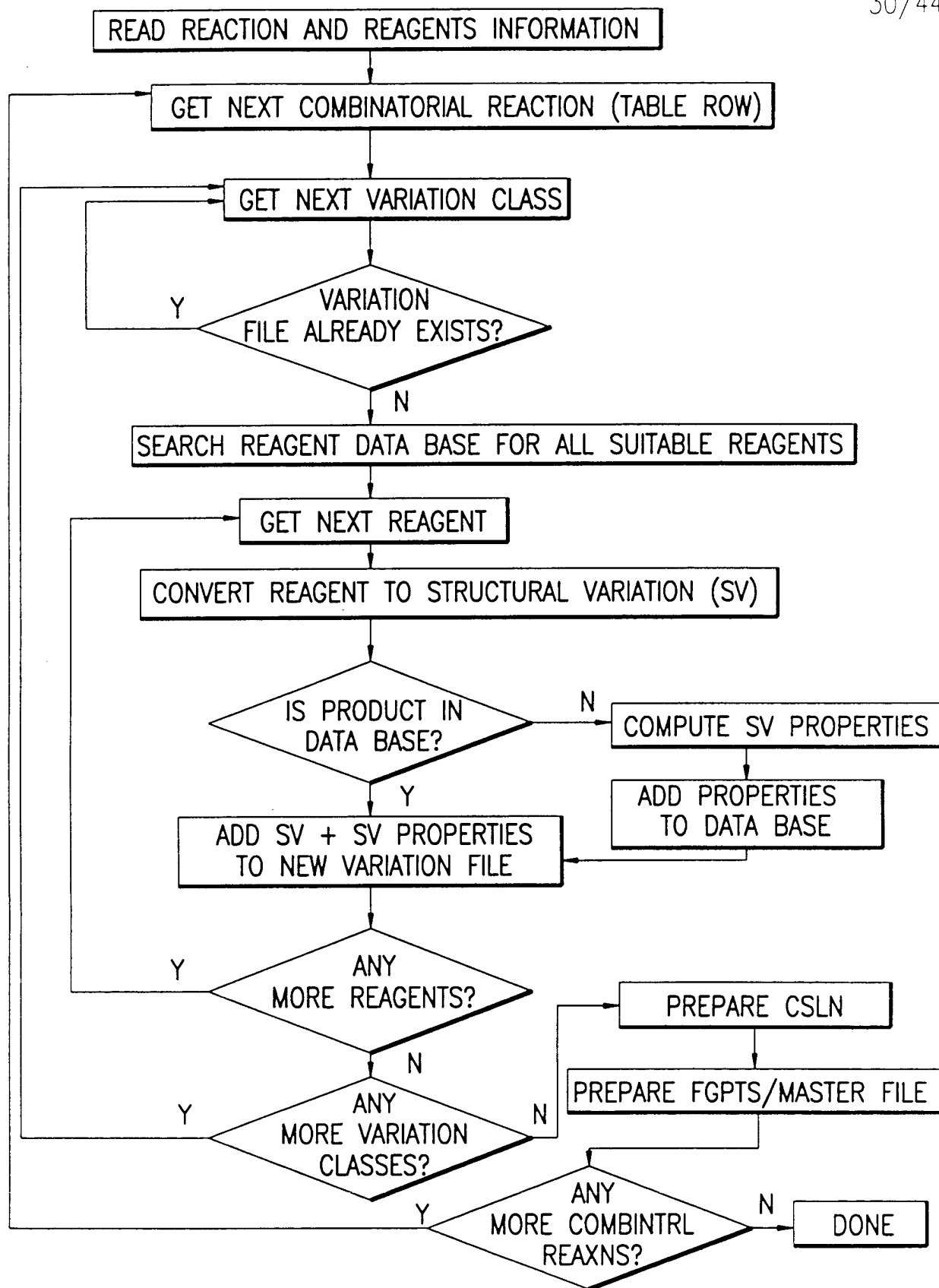


FIG.17

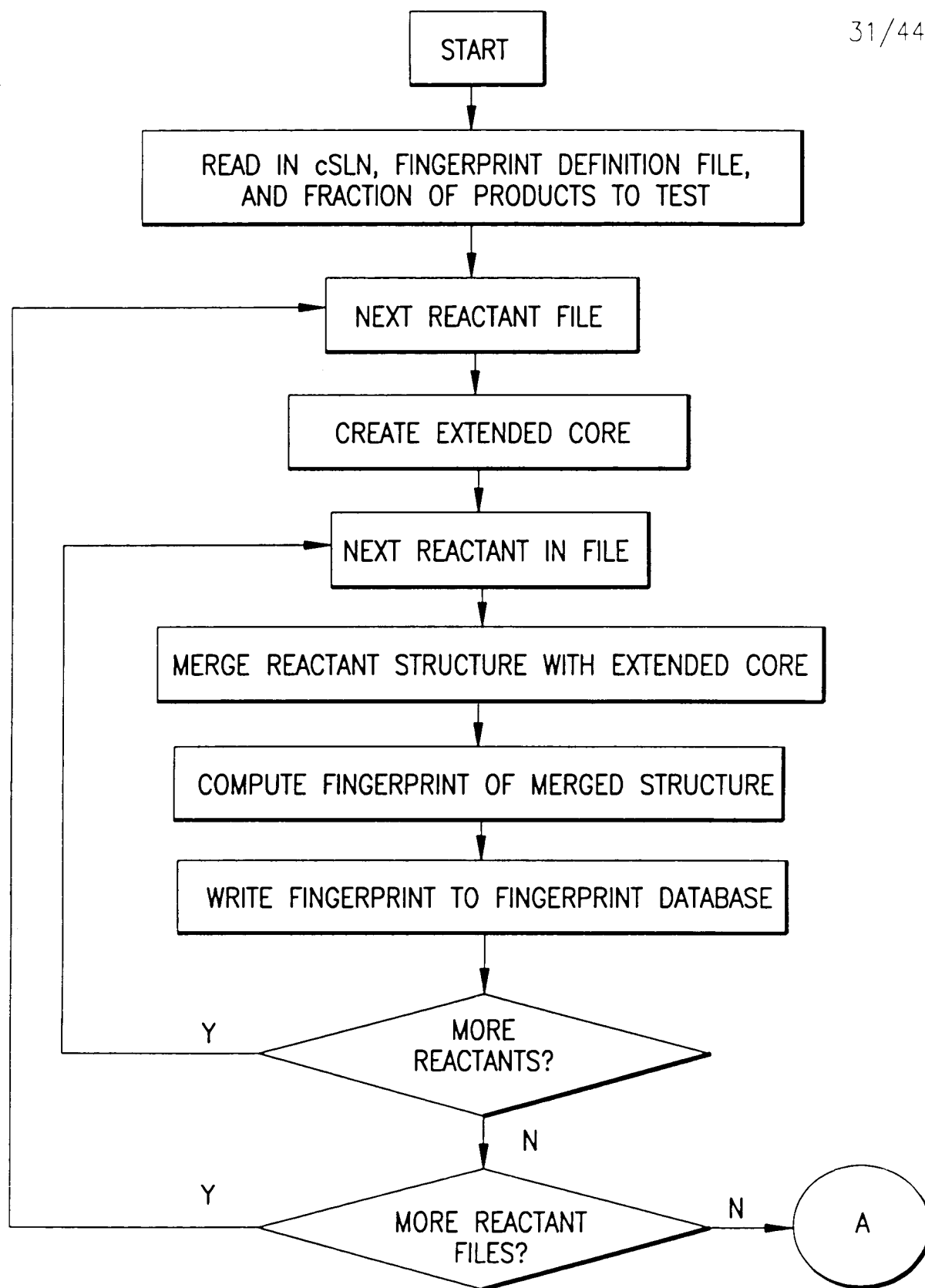


FIG.18

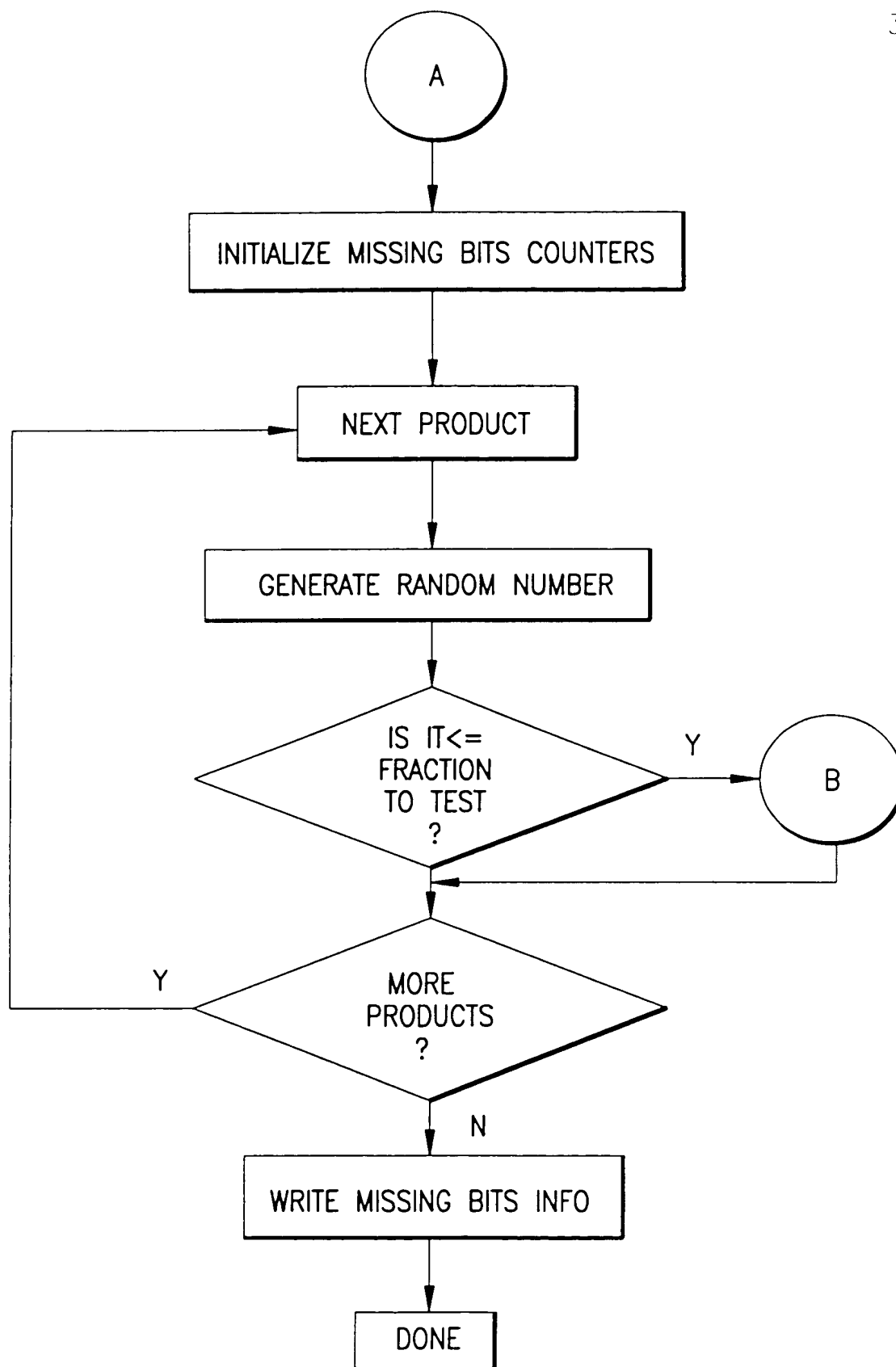


FIG.19



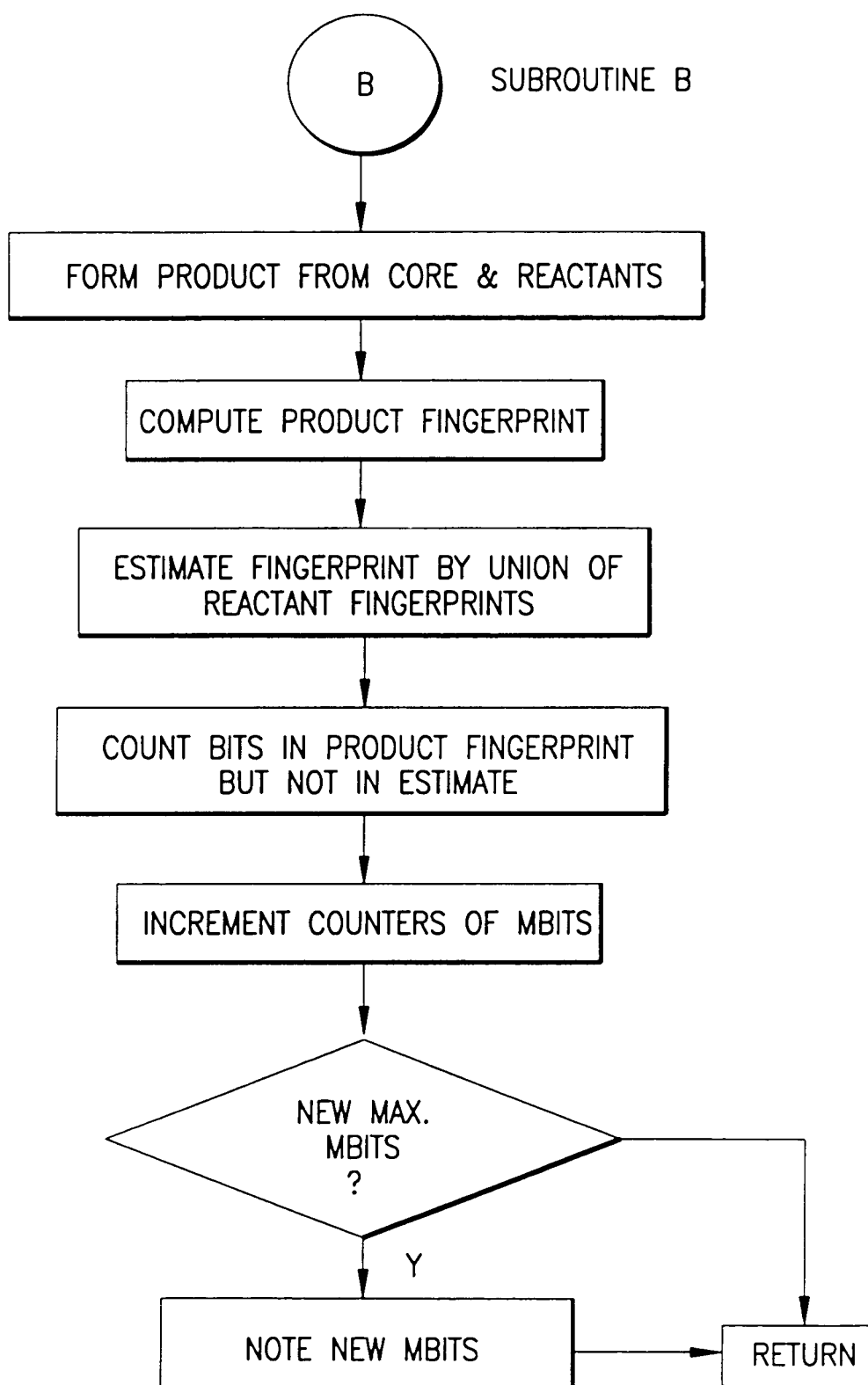


FIG.20

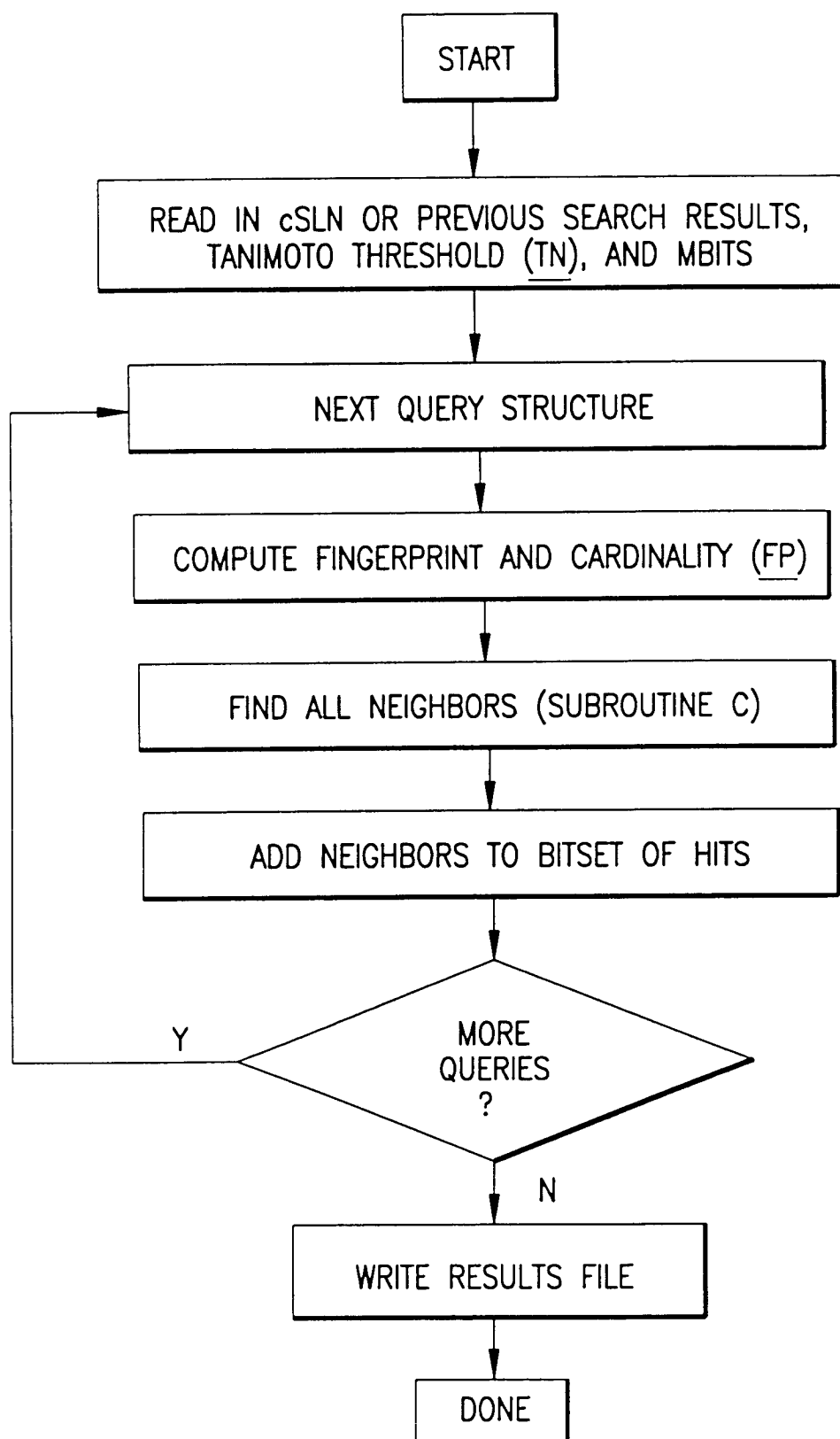
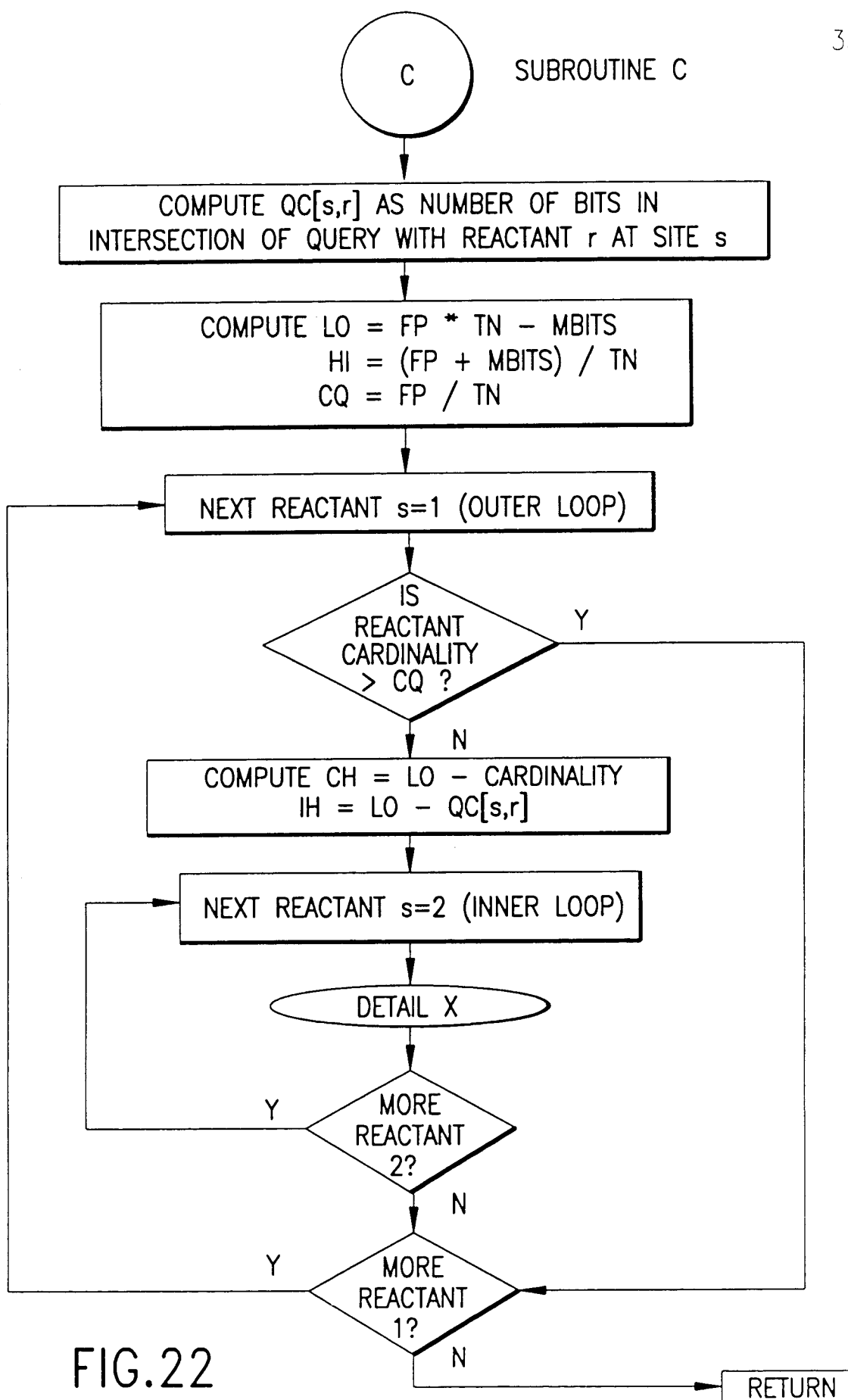


FIG.21



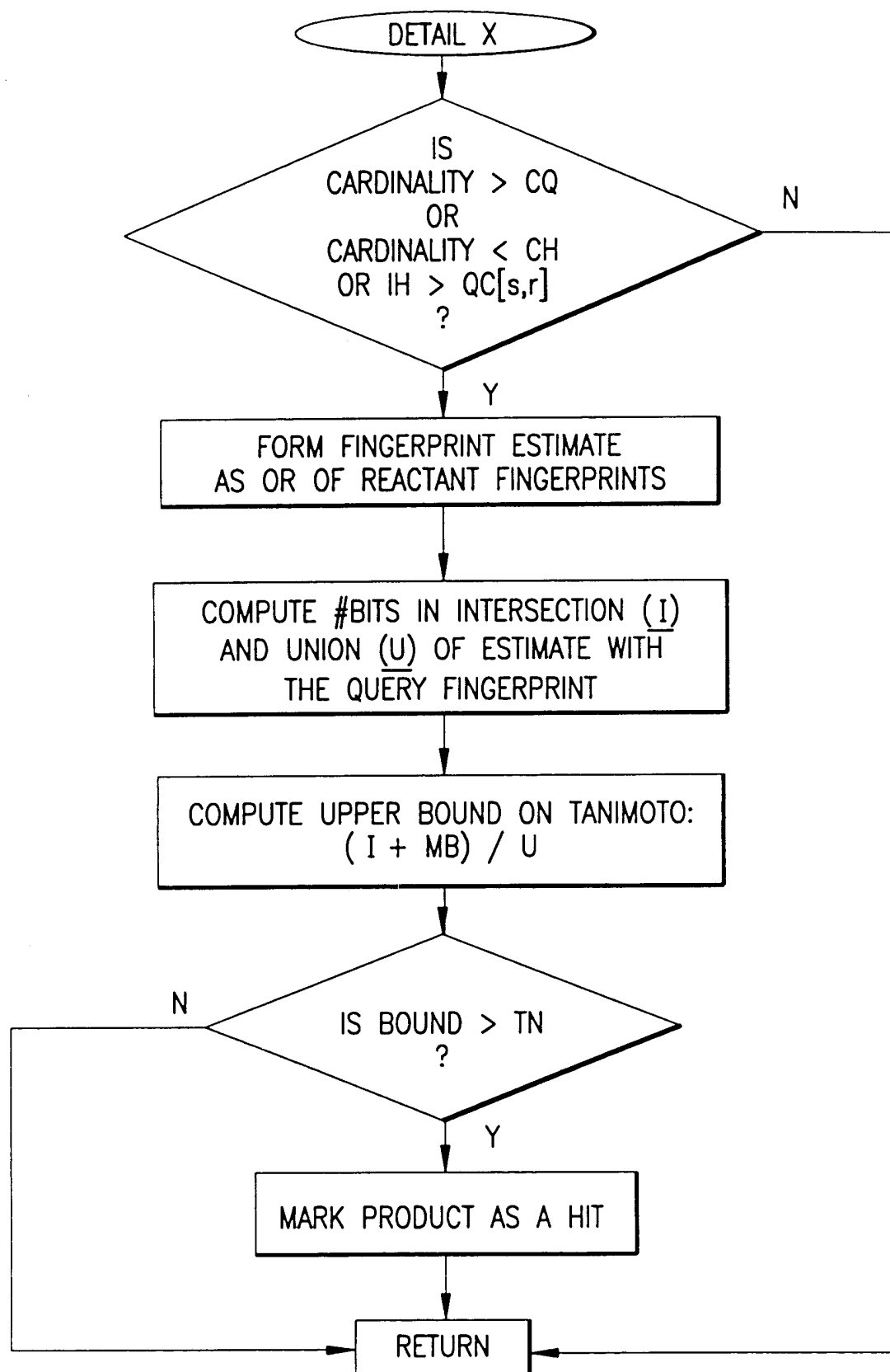


FIG.23

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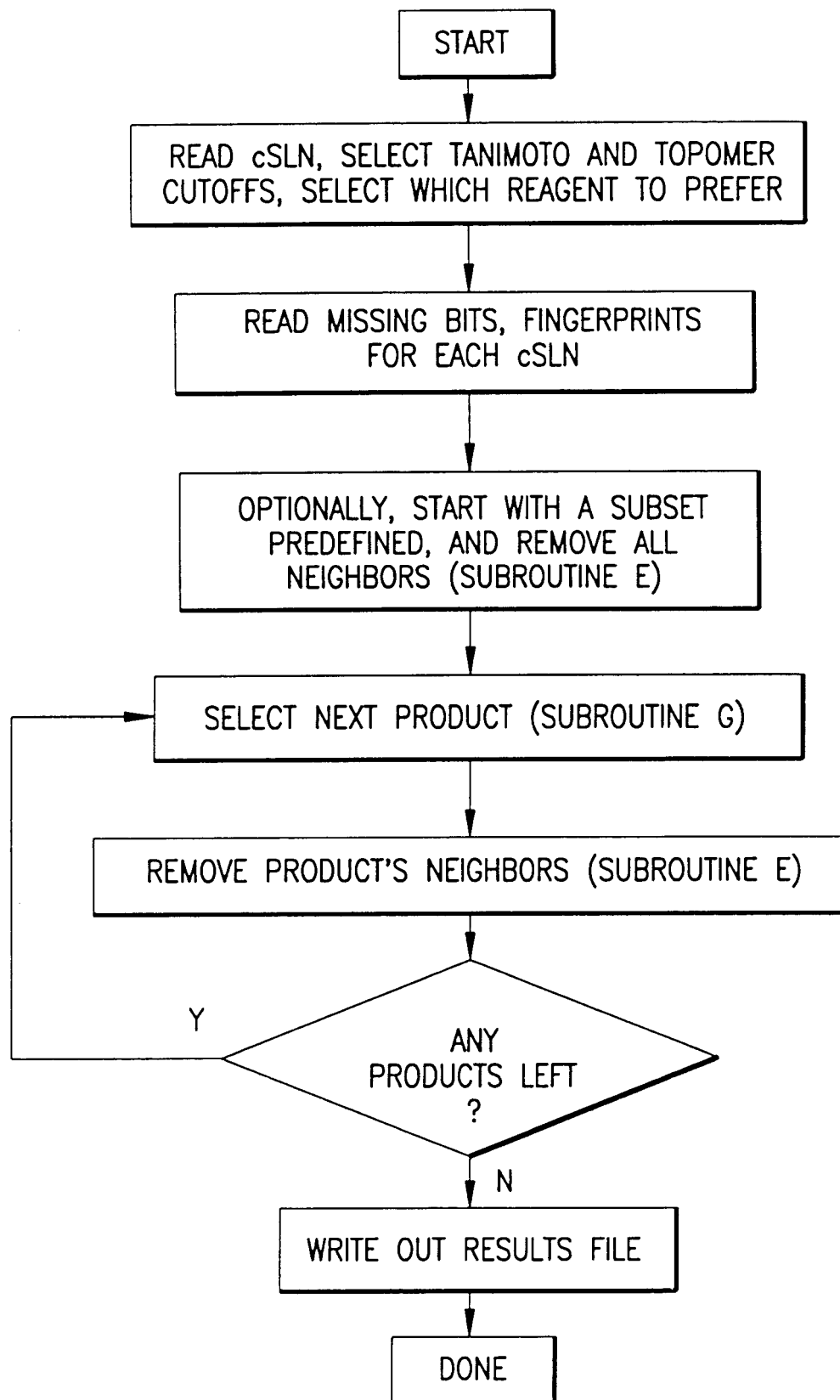


FIG.24

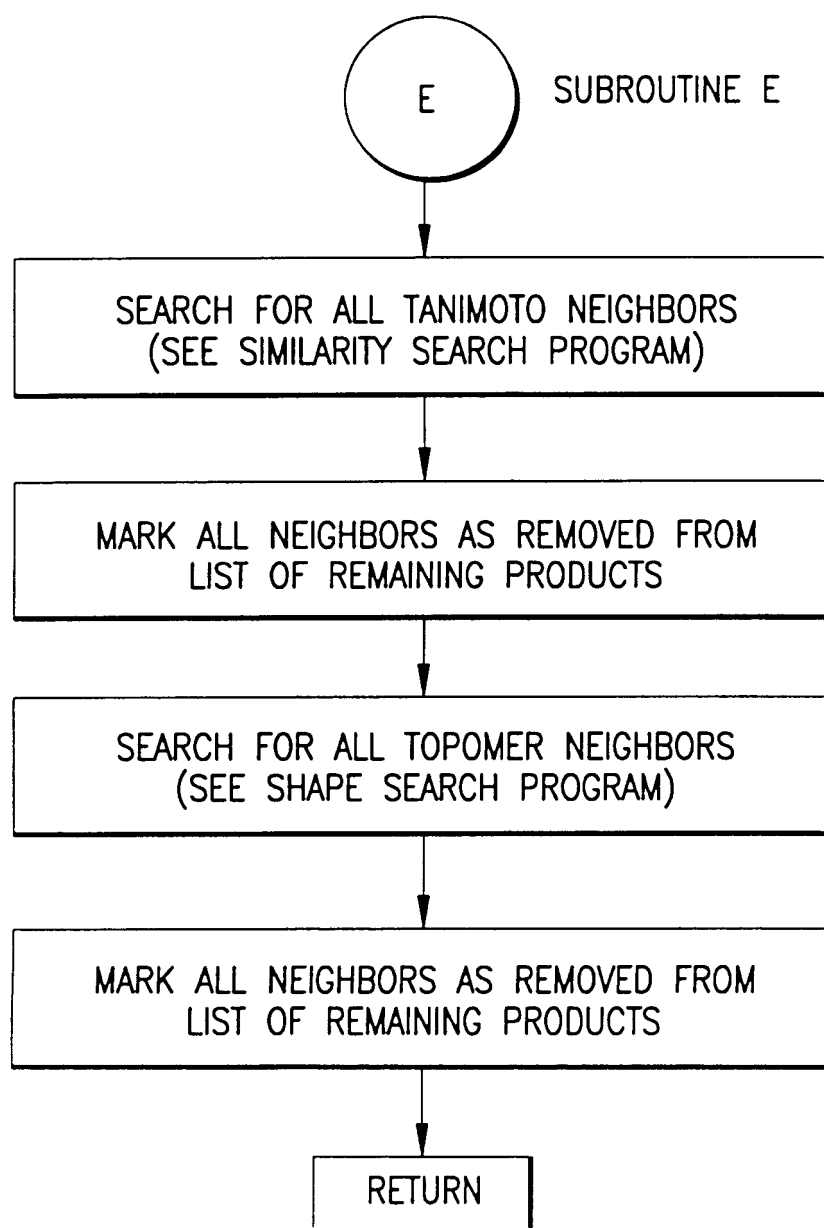
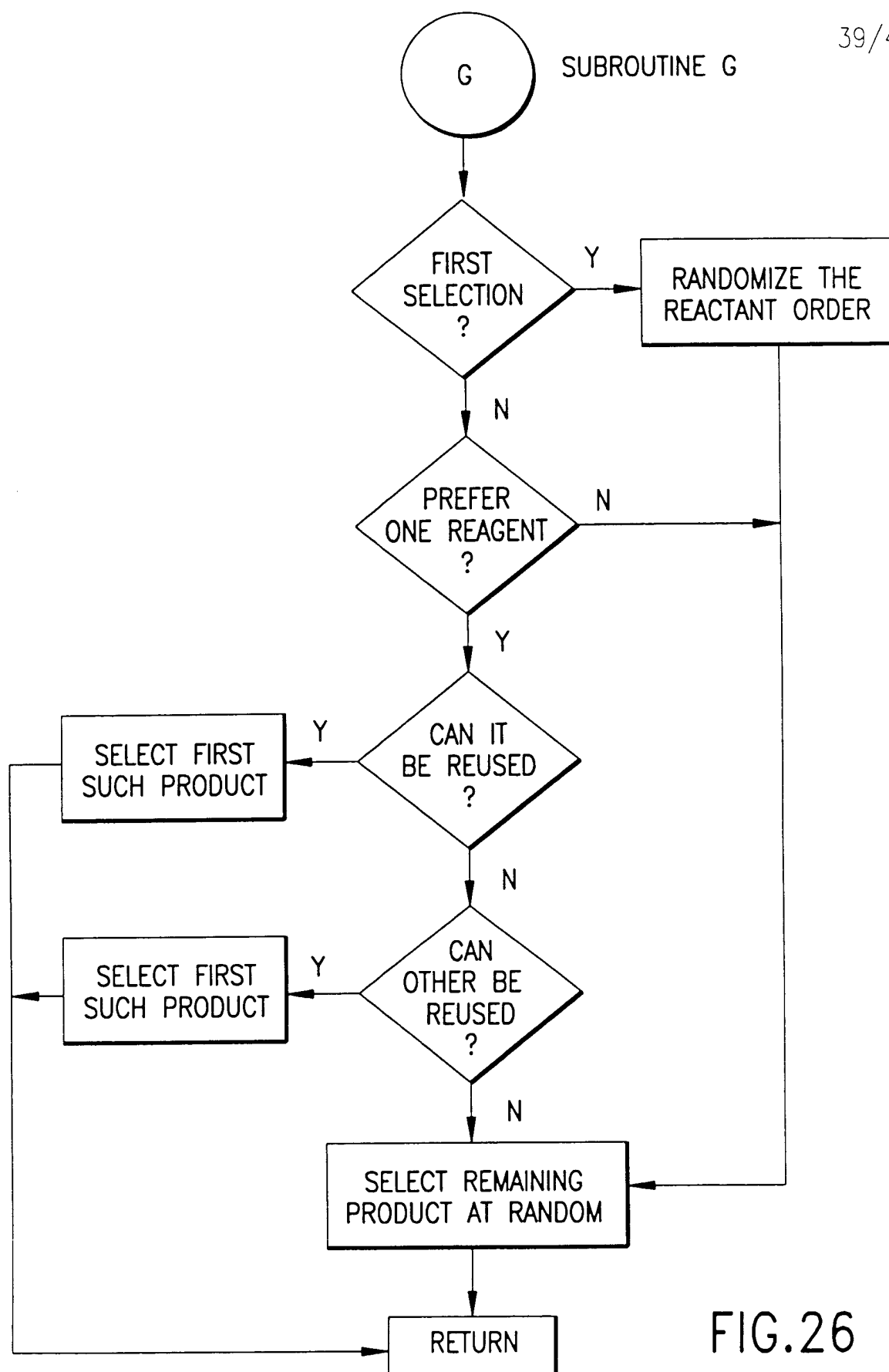


FIG.25



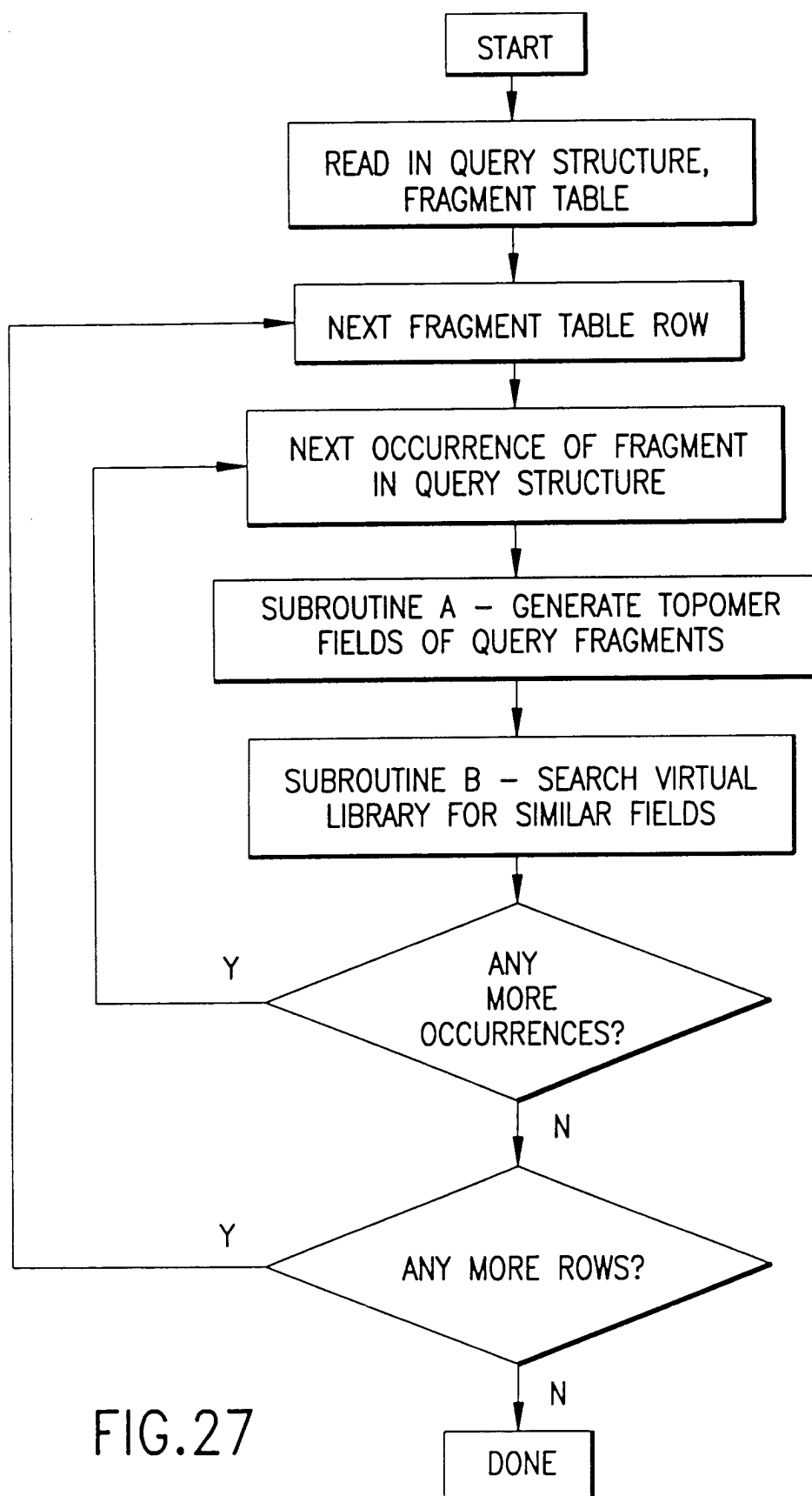


FIG.27



## SUBROUTINE A

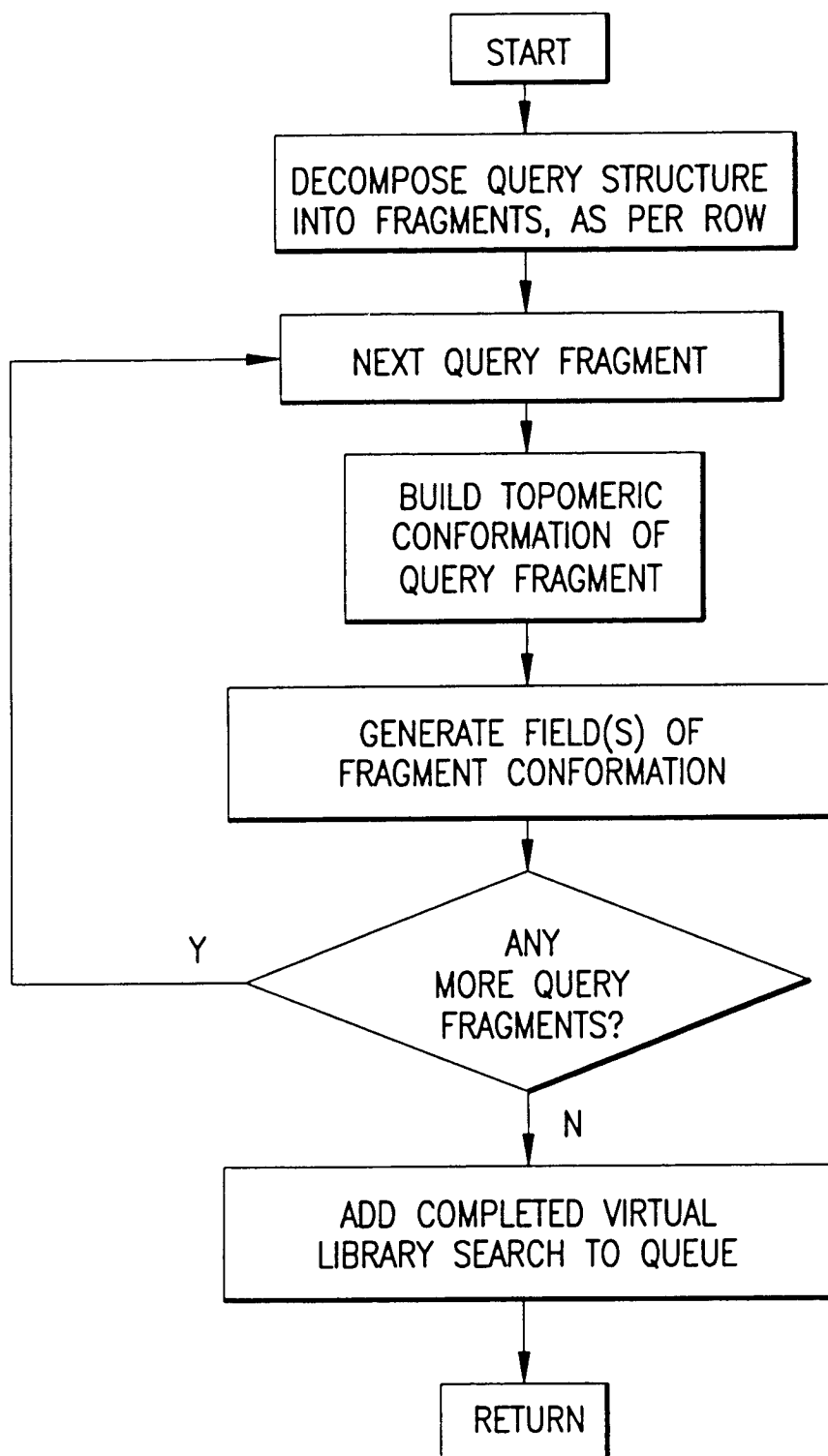
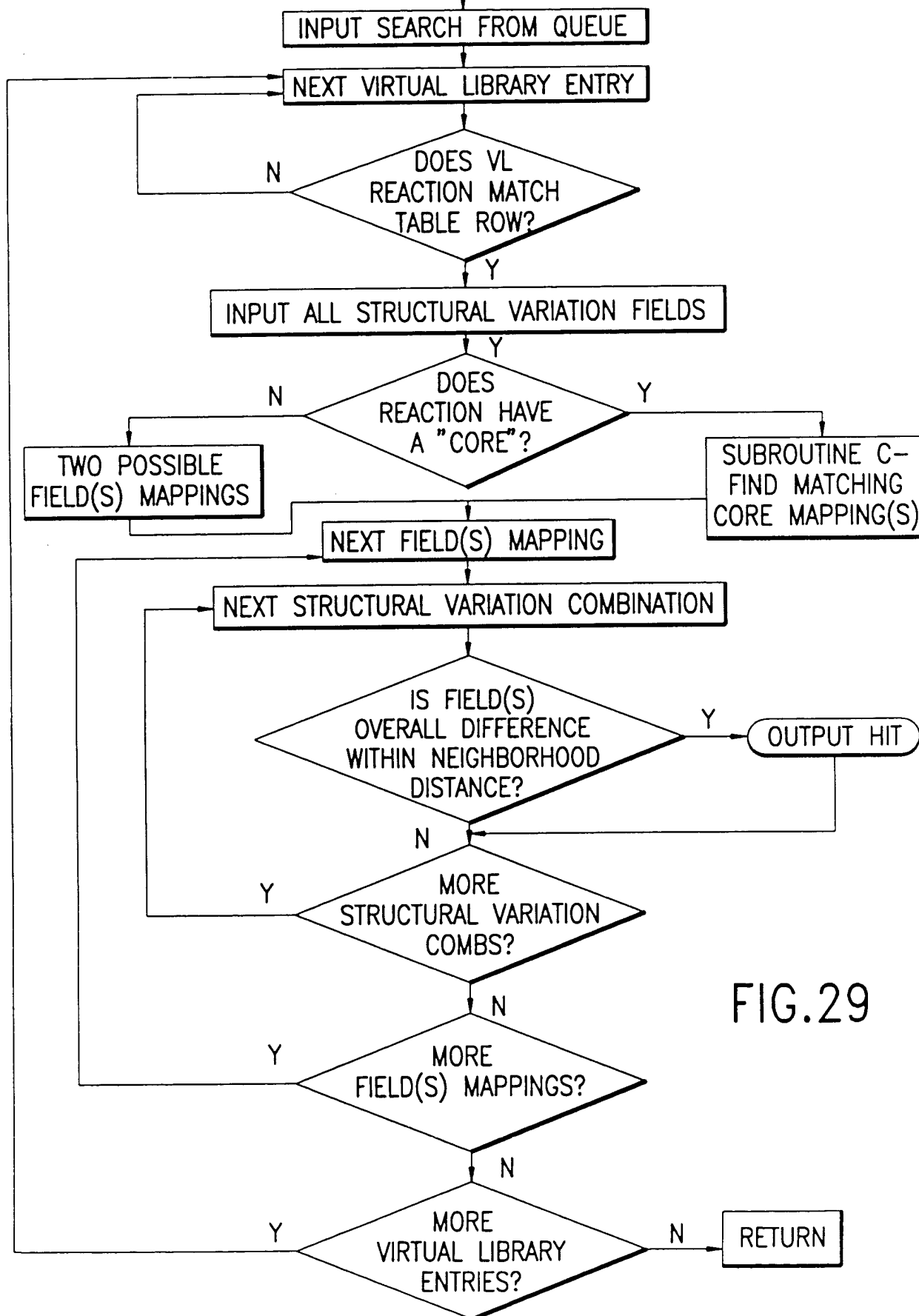


FIG.28



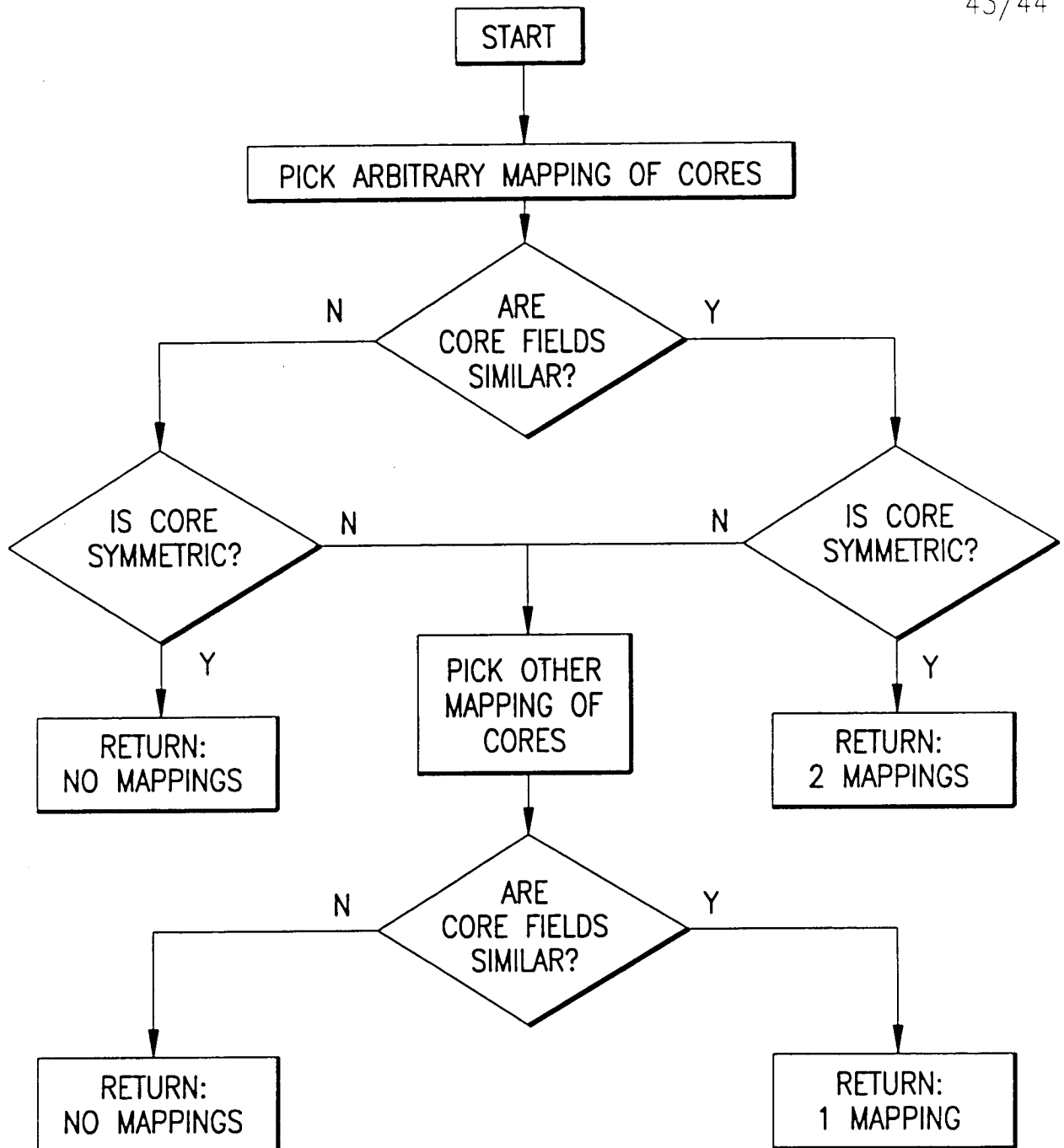


FIG.30

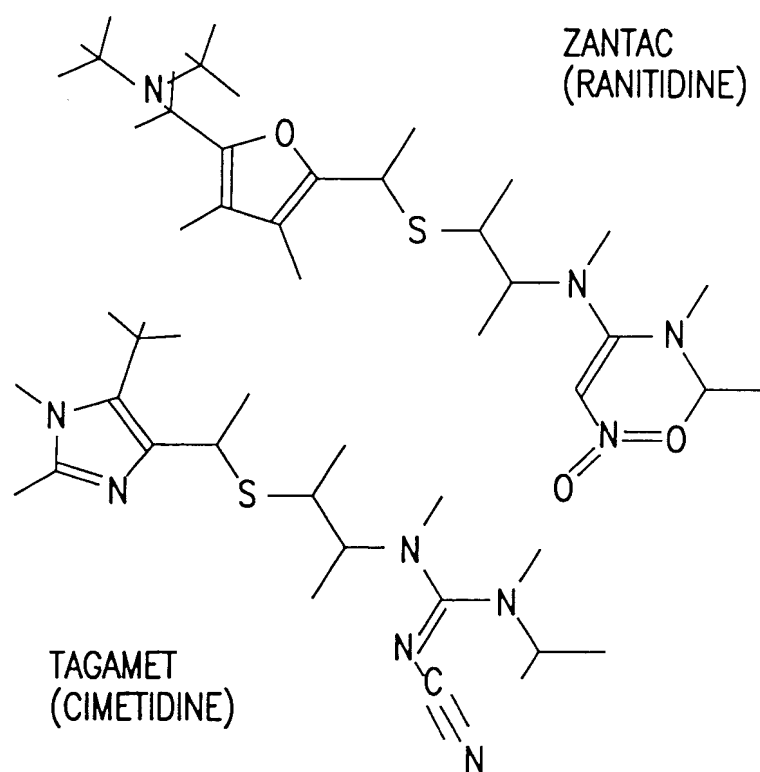


FIG.31